Skills Gaps in Physical Chemistry and Its Oceanographic Applications, and Needs for Capacity-Building

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This community consultation is a joint initiative of the **Ocean Carbon and Biogeochemistry Project Office** (sponsored by the *US National Science Foundation* and *National Aeronautics & Space Administration*) and the Chemical Speciation Task Group of the **Joint Committee on the Properties of Seawater** (sponsored by the *Scientific Committee on Oceanic Research*, the *International Association for the Physical Sciences of the Oceans*, and the *International Association for the Properties of Water and Steam*).

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Summary

There is widespread concern amongst oceanographers about dwindling expertise in the physical chemistry of natural waters (e.g., acid-base speciation, trace metal complexation, and mineral solubility) that is so foundational to the field of chemical oceanography, including constraining the ocean carbonate system and bioavailability of micronutrient trace metals. We have therefore polled a broad swath of the international ocean science community to assess perceived levels of preparation and competence in these chemistry fundamentals. We received 104 responses to our survey, and additional feedback via email from representatives of a number of international programmes and networks. This report includes a summary of the responses we received, and a compilation of the survey demographics and detailed comments from respondents.

In addition, to facilitate community and capacity building, we sought feedback on the idea of convening an international workshop to bring together chemical oceanographers across sub-disciplines and career stages with leading scientists from other fields with relevant expertise (e.g., physical chemistry, aquatic geochemistry, chemical engineering, etc.) to engage in scientific discourse and exchange ideas, develop new collaborations, and formulate new curricular and capacity building tools. Such an activity could generate new initiatives in training and research in physical chemistry measurements and models for applications in oceanography.

The purposes of this document are: (1) To summarise the results of the survey, and the ideas of the international oceanography community for addressing the identified skills and capability gaps, and their effects. (2) To support a future application, after consultations with possible sponsoring organisations, for a workshop to assess current skills and capability gaps, their effects, and identify how best to address them.

The key findings of the survey are as follows:

- Numerous respondents noted a skills gap in the fundamentals of physical (both thermodynamics and kinetics) and analytical chemistry, particularly as it pertains to the ocean carbonate system, including the development and application of chemical speciation models. There is concern about the use of these models as black boxes without understanding their origin and limitations. This is especially concerning amidst the recent uptick in marine carbon dioxide removal (mCDR) research and field trials.
- Many noted that undergraduate and graduate-level training in chemistry is inadequate, and that many scientists enter the field of chemical oceanography with a broader background in biogeochemistry and environmental science. Students are getting less hands-on analytical training and experience, and many are using existing or autonomously collected biogeochemical datasets. These views were shared across career stages, from graduate students to senior academics.
- Respondents recommended several high-priority focus areas for capacity building, including (but not limited to) organic alkalinity, coastal and estuarine carbonate chemistry, metal cycling, organic metal complexation, calibrations and standards for pH and other quantities, sediment porewater chemistry and speciation, electrochemistry, ocean sediment and alkalinity interaction, and chemical weathering.

- In addition to a workshop, respondents suggested model and laboratory intercomparison work, summer schools, instrumentation training, and activities that bridge physical chemistry experimentalists with those who build and use models.
- Limited access to analytical capabilities, training, and materials presents a major barrier for scientists in developing countries and should be given careful consideration in planning future capacity building activities and training materials.

We also expressed our concerns to the following oceanographic organisations and sought support for the idea of an international workshop: **SCOR** (*Scientific Committee on Oceanic Research*), **IAPSO** (*International Association for the Physical Sciences of the Oceans*), **IOCCP** (*International Ocean Carbon Coordination Project*), **GEOTRACES** (*An International Study of the Marine Biogeochemical Cycles of Trace Elements and Isotopes*), and **SOLAS** (*Surface Ocean – Lower Atmosphere Study*). They have all replied positively, and their responses are included here.

In the remainder of this document, we first describe the demographics of the respondents (career stage and country of origin) and then present the compiled responses to our proposal of a workshop followed by the training and research needs identified by respondents. **The number at the beginning of each response refers to the respondent's geographic region.**

1. Introduction

The survey announcement and solicitation for information to the international chemical oceanography community is reproduced in Appendix 1. It states the nature of the capacity and "skills gap" problem, and possible steps towards addressing it beginning with a workshop to define needs. This document compiles the responses entered in the survey in answer to these requests:

1. *Please share any feedback and/or ideas you have about skills gaps in physical chemistry and its oceanographic applications and needs for capacity-building*.
2. *Please share any ideas or feedback you have on networks or contacts we should engage in this community endeavour*.

We have organised the responses to request (1) above by subject area. A few responses cover more than one area and have been split up. Where this has been done, there will be a '…' in the text.

The number at the beginning of each printed response in this document is a reference number that identifies the sender (that information is not presented here). However, the following table can be used to determine the country or region of origin of the response:

Table 1. Countries and regions corresponding to the reference numbers of all responses

Country/region	Reference numbers		Country/region	Reference numbers
US and Canada	1-44		Russia	91
Central and South America	45-51		Africa	92-93
United Kingdom	52-66		Far East	94-99
Other Europe	67-84		India/Pakistan/Bangladesh	100-104
Australia/New Zealand	85-90			

We also approached several international oceanographic organisations to ask whether they agree with the ideas expressed in our solicitation and support the idea of a workshop (Section 3, and Appendix 3).

Sections 4-8 contain the responses of individuals. The ordering of responses within each section is not significant. Appendix 2 contains a communication concerning the needs and perspectives of Southeast Asia, from which we had a relatively small response.

2. Survey respondent demographics

These statistics include only the individuals who entered their responses on the online form. We also received a few replies by email. Responses were well distributed across career stages:

Table 1: Career stage of individual responders

No.	Career stage	No. of responders	Percentage of total
1	Student/postdoc	27	26
2	Early (5-10 years post Ph.D)	29	27.9
3	Mid (11-20 years post Ph.D)	26	25
4	Late (>20 years post Ph.D)	22	21.1

The countries and regions of origin of the respondents (or, strictly, those of the institutions to which they are affiliated) are listed in Table 2:

Table 2: Locations of individual responders

Country or region	No. of responders	% of total
US and Canada	44	42.3
Central and South America	7	6.7
UK	15	14.2
Other Europe	18	17.3
Australia, New Zealand	6	5.8
Russia	1	1.0
Africa	2	1.9
Far East (China inc. Taiwan, Japan)	6	5.8
India, Pakistan, Bangladesh	5	4.8

Finally, the declared expertise of the respondents is listed below. Many individuals had expertise in more than one area. The top four areas of expertise are marked in bold red. Respondents from North America (USA and Canada) have a particular interest in marine carbon dioxide removal (mCDR).

Table 3: Numbers of responders with expertise in each of the areas of research activity. The top four items are bold red.

	Expertise and interests	All regions	North America	All Europe	UK only
1	chemical oceanography/aqueous geochemistry	**34**	**18**	**9=**	**7**
2	ocean carbonate system	**63**	**35**	**15**	**6=**
3	trace metals	**43**	**17=**	**13**	**6=**
4	paleoceanography	17	6	**9=**	4
5	chemical engineering	3	3	-	-
6	mCDR	27	**17=**	6	2
7	laboratory measurements & instrumentation	**71**	**30**	**27**	**11**
8	chemical sensors	25	15	6	4
9	standards and reference materials	21	11	**9=**	**5**
10	speciation models	16	10	5	3
11	metal isotope geochemistry	1	1	-	-
12	biogeochemical and earth system models	3	1	2	2
13	data product development	6	1	3	1
14	marine silica cycle	1	1	-	-
15	bio-inorganic chemistry	1	-	-	-
16	cycling of amino compounds, volatile amines	1	-	1	1
17	nutrient chemistry	1	-	1	1
18	chemical tracer hydrology	1	-	-	-
19	project management	1	-	-	-

3. Support for the idea of a workshop (international organisations)

We proposed holding an international workshop to bring together chemical oceanographers from different sub-disciplines with leading scientists from other fields with relevant expertise. Its purpose would be to: (i) identify subject areas within chemical oceanography that are impacted by the lack of physical chemistry skills in both modelling and experimental methods; (ii) define what is needed to address this skills gap and where (in other areas of chemistry, geochemistry, and chemical engineering) these skills can be found.

The following organisations were approached and asked for their opinions of the value of a Workshop, and their responses were as follows:

- **IOCCP** (*International Ocean Carbon Coordination Project*)
  Response: The proposed workshop and future capacity building are very important and timely activities. IOCCP offers to support the community, in whatever ways it is able, to help ensure that this initiative goes ahead.
- **IAPSO** (*International Association for the Physical Sciences of the Oceans*)
  Response: IAPSO will endorse, at least in terms of giving a symbolic stamp of approval but without financial commitment yet. Should the time come, it will be re-assessed.
- **SCOR** (*Scientific Committee on Oceanic Research*)
  Response: the Workshop is a good idea and there was agreement with the five key points identified in the concept note. There was also a suggestion to explore low-cost affordable instruments and practices to engage developing countries, given the capacity building component of the proposed workshop, and also to link to policy in order to enhance the value chain of chemical measurements to develop indicators for monitoring and management purposes. This might be an opportunity to invite other expertise such as MPA managers and IOC staff.
- **SOLAS** (*Surface Ocean Lower Atmosphere Study*) – see letter of support (Appendix 3)
- **GEOTRACES** (*An International Study of the Marine Biogeochemical Cycles of Trace Elements and Isotopes*) – see letter of support (Appendix 3)

4. Support for the idea of a workshop (survey respondents)

Using a survey – a Google form distributed to OCB, SCOR, GEOTRACES, IOCCP, Marine Chemical Speciation (MarChemSpec), and other ocean science networks - we queried members of the oceanographic community about the idea of a community workshop as described above. The responses were positive, and detailed respondent feedback is included below. The **bold** text is used to highlight key points and ideas that were expressed multiple times.

32. I couldn't agree more with the need for a workshop like this. Perhaps adding an **electrochemistry** component to the workshop would facilitate students making connections between redox, electron transfer reactions, speciation. Other topics that need more attention: general application of **kinetics** coupled to thermodynamic equilibrium, general inorganic chemistry concepts of molecular orbitals and geometry of molecules; careful application of adsorption models

33. Yes, agree with all premises for this workshop. I would suggest extending the topic from chemical oceanography to include **chemical weathering** (i.e., water-rock reactions in terrestrial and

marine systems) -- essentially part of the same system as that addressed by 'chemical oceanography' and equally relevant to paleoceanography/mCDR/ocean carbonate chemistry. There seems to be a growing deficit in competency in this area, as well.

36. This is a critical effort for maintaining and increasing knowledge of physical chemistry as it pertains to chemical oceanography. I support a workshop to bring this type of knowledge back to the forefront and encourage discussions amongst early careers with those more established in the field. I believe there is a **distinct gap between those studying physical chemistry of seawater whose research utilizes experimental methods and those using modeling. I think it would be especially important to try to bridge this gap.**

42. I think this is fantastic, I keep seeing people working on **mCDR** that don't understand the physical chemistry and are oblivious to what should be obvious problems/challenges to experiment design and methods.

63. I'm completely supportive of this effort and enthusiastic about being engaged (and helpful if at all possible). One aspect of the problem might stem from teaching, in that these important topics don't figure in many physical chemistry courses I am familiar with (at least those based in Chemistry Departments in the UK), while **the way aqueous geochemistry is taught, if at all, tends to emphasise applications rather than develop a deep understanding of the fundamentals** - more as a means to an end. I think there is potential to pull in a lot of chemists residing in Chemistry Departments to contribute to building capacity. Perhaps a community-sponsored short course (or series of short-courses) might provide motivation to address this.

65. Thanks for organising such an important workshop. Ideas:

-**Specific workshops for ECRs** to build up training in relevant analytical techniques

-An event to discuss data **QC techniques** relevant in Chemical Oceanography

-A **best practice handbook** for data QC would be useful to avoid publication of low-quality data.

66. Good idea to team up with existing programmes such as the GEOTRACES **Summer School** (which does already offer some relevant workshops) to gain access to students/postdocs and provide foundational training at an early career stage. Shared, or recommended, learning and teaching resources to ensure the same key concepts are taught across the board.

83. Organising **summer schools** might be a good avenue

96. This workshop will be important for the future GEOTRACES! Increase our capability of the simple methodology, **shipboard analytical methods**, exchange the knowledge/training the existing method.

5. Skills gaps and training needs

Here, we compiled the **most relevant responses concerning gaps in skills and abilities**, answering request #1, first from senior staff (reporting what they see in students and postdocs) and then the views of the younger staff as to their needs.

(a) Views of senior faculty and staff

(email, USA). I'm excited about your initiative. I've been concerned about the same issues for a long time. There are some **fundamentals about the physical chemistry of seawater** that students need to learn.

6. I agree with the all the concerns raised. I perceive a distinct lack of fundamental understanding among recent student cohorts. My program is part of the problem, we do not currently teach any course which addresses the developing knowledge gap. **Students are taught large-scale biogeochemical cycles but are unable to do any fundamental calculations**. In the few cases when students are shown the calculations underpinning processes in the ocean, e.g., the ocean carbonate system, too little time is allocated. And/or the **students lack the preparation to understand the physical chemistry**.

8. The **skills gap in physical chemistry mirrors that of physics and mathematics in general within oceanography among younger scientists**. This suggests that students are not getting this training from an early stage. I am unsure about the root causes of this. Maybe students feel studying these ideas and learning these skills is unnecessary, or uninteresting. But I think it requires serious rethinking of how and what we teach.

13. **Not many students or early career scientists are familiar with or perform direct measurements of CO2 system parameters**. This was something that became more apparent at Ocean Sciences 2024. Many people are starting to focus on mCDR or OAE or analysis of previously collected measurements /float data. I am not sure if this is beyond the scope of this project, but I am possibly incorporating some of those concepts and showing researchers how physical chemistry applies to these new fields.

24. Many people expressed concern as **many young scientists are now being trained more to use data rather than collect data** and how **not many groups are actually performing CO2 system measurements in the lab**. We do not want to lose experts on CO2 system measurements

28. I feel that a solid background in the physical chemistry of seawater is an essential core component of students training. It may not be where the most important new research is taking place but it is important for understanding the processes and reactions in seawater that we use on a daily basis. Just to illustrate using one example: **the concept of chemical potential for ions in solution and how activities of ions are defined is not usually taught in core Chemistry Dept. or Chemical Oceanography courses**. This and other core principles should be included in our education.

31. I'm interested in resolving the inconsistencies in the marine carbonate system by combining thermodynamic principles and rigorous Bayesian data analysis. **It is difficult to find students interested in the marine carbonate system that have training in basic physical chemistry and mathematical modeling.**

52. I've worked in a marine science technical/analytical chemistry role for 15 years. We find replacing key experienced staff increasingly difficult - less applicant who **don't have much practical ocean chemistry/analytical experience**). We have a very limited/no training or additional wage

budgets to train up in-house technicians/staff. Little interest from applicant with knowledge/skills of a broad range on bench and analytical chemistry.

54. **Not sure if it's a skills gap or just an awareness gap. I don't think Ocean Science is an area that is actually known about**, let alone considered, by pure chemists, we never have applications from them for our studentships or jobs.

(b) Views of students, postdocs, and young faculty

16. **Carbonate chemistry stands out to me as a major knowledge/skill gap** at my career stage (students/postdocs, even some early faculty). I've interacted with lots of folks who **treat carbonate chemistry solvers as black boxes** - without understanding how they work or which variables might matter for their calculations - and unfortunately end up with a different result than they wanted. This seems especially prominent and problematic in the growing mCDR field, where accurate carbonate chemistry calculations make a big difference.

18. I have just started as an assistant professor and will be teaching graduate level chemical oceanography and aquatic chemistry next year. As a brand new professor, I am not yet as aware of gaps in the next generation's knowledge as more established professors might be, but I am very interested in **building the aqueous chemistry community**, sharing educational resources, and generally getting involved in the topics this workshop addresses. For example, I am eager to come up with helpful and engaging exercises for my aquatic chemistry students that will help them grasp difficult concepts, and it would be very beneficial to me to have a network of colleagues or collection of resources I could draw on to design the best problems, assignments, and syllabus I can.

40. While there are a handful of people with high level of expertise in this subject, there is very obviously a large and **growing gap of skilled knowledge surrounding chemical speciation**. This work is foundational to my PhD project and likely to projects I will work on in the future. It would be nice to both deepen my own understanding as well as have a larger community to work with when exploring this topic.

88. A **lack of training in general chemistry** is common in students in Australia. **Many students enter this field from broader environmental science backgrounds but lack chemical expertise**. This knowledge deficit pertains to acid-base chemistry, metallic complexation and ligands, instrumentation and separation chemistry. As a PhD student in this field, I feel that the gap between environmental or applied science and biogeochemical concepts may be due to a **lack of students engaging in straight chemistry. This might be due to reduced engagement in chemistry in undergraduate courses**, or a lack of training during post-graduate courses prior to the PhD realm.

91. **I would like to learn more about the intricacies of calculating CO2 solubility constants** for regional estimates of exchange at the water-atmosphere interface. And also about related measurements of CO2 fluxes using different methods and their comparison.

6. Training and research needs by subject area

These are listed below. Our solicitation identified the carbonate system and mCDR as two specific areas of concern, so perhaps it isn’t surprising that many responses were focused on the science of these topics.

(a) Carbonate system

10. I have only dabbled lightly in CO2 chemistry as was a relatively small part of my work where I mainly focused on hydrodynamics, I am however really keen to learn more to expand my **numerical models** and include various other chemical interactions.

12. **Organic alkalinity**, hypersaline conditions, colloids and nanoparticles.

15. Development of best practices for **coastal/estuarine carbon system measurements**!!! Including unidentified sources of TA

19. For the marine carbonate system measurements, our knowledge on **organic alkalinity** is still lacking. And it plays an important role in estuaries and other particular regions, which sometimes lead to inconsistencies between measured and calculated TA. Involvement of new instruments and technics may help us to understand this topic, such as LC-MS, Orbitrap-MS from analytical chemistry. This parameter should also be considered in building models such as MarChemSpec, CO2SYS, etc…

20. I am particularly interested in developing **calibrations and standards for pH and other quantities**; resolving uncertainties and inconsistencies in the relationships of the parameters of the marine carbonate system; and chemical speciation models in **low salinity water and organic alkalinity** in brackish to low salinity waters.

26. As a chemical oceanographer specializing in carbonate chemistry, I'm starting on research to explore the impacts of **high alkalinity** on various ecosystems. Currently, there's a deficiency in fundamental understanding regarding the dissolution of various minerals, metal speciation across different pH levels, and their effects on diverse biological processes (from individual to ecosystem scales). In addition to the development of SOPs and methods to measure these processes in the lab and in the field.

Here are some thoughts on skills gaps and capacity-building needs in this area: Understanding and predicting how changes in pH and alkalinity affect chemical equilibria and kinetics in seawater requires a strong background in physical chemistry, particularly in **thermodynamics and reaction kinetics**. A capacity building activity could include the development of specialized courses and training in **marine chemical modeling**, including the use of software and coding skills necessary for developing and running these models. Strengthen interdisciplinary training that combines physical chemistry with marine biology and environmental toxicology to understand the impacts at the organism and ecosystem level.

27. Carbonate system, equation of state of seawater and basic marine physical chemistry have serious gaps in skills. Coincides with the **demise of aquatic chemistry as a discipline** in Environmental Engineering Departments.

35. Bridging the **limnology-oceanography divide** w.r.t. carbonate equilibrium

45. **CRM for coastal waters, pH techniques/protocolos for coastal waters** with high variability and productivity (pHt sometimes is not apply to this waters)

62. The need to improve and better standardise carbonate chemistry calculations is something my group and others in the paleo CO2 community have been working on fairly concertedly in the last

few years. We've been trying to make sure the workflows used to make CO2 system calculations are robust between different software in different coding languages. This has involved extensive testing under modern seawater conditions and also under conditions of altered major ion chemistry (e.g. Ca, Mg, SO4). From this we've identified a number of ways in which calculations might be streamlined or improved.

This follows on from work I did within my PhD trying to standardise different CO2 system calculation methods, which led to co-authorship on CO2SYS, and bug fixes in csys, ODV, and seacarb.

67. **Resolving uncertainties and inconsistencies in the relationships of the parameters of the marine carbonate system**, and the need for consensus best practices and reference materials.

72. There is a significant knowledge gap regarding the origin **of inconsistencies between measured and calculated values of the seawater carbonate system**, particularly with regard to pH. This is preventing the enhancement of internal consistency between variables, laboratories and countries. Given the importance of ocean acidification estimates, which are currently based on trends estimated from either measured or calculated values, it is crucial to address this knowledge gap, especially for future scenarios where ocean alkalinity enhancement may be a reality.

76. Resolving **uncertainties and inconsistencies in the relationships of the parameters of the marine carbonate system**. Total alkalinity (TA) is one of the four main carbonate system variables measured to describe marine water carbonate chemistry, as well as an important indicator of the ocean buffering capacity, as well as a measure of its capacity to resist acidification. Historically, TA is primarily associated with the inorganic components of seawater such as bicarbonate, but there is a growing concern in the marine scientific community that dissolved organic matter (DOM) can significantly contribute to TA in coastal waters. This organic fraction of TA (OrgAlk) is typically considered negligible and is not accounted for in conventional TA equations.

However, omission of **OrgAlk** can lead to the propagation of errors in carbonate system calculations and to misinterpretation of air–sea CO2 flux, degrees of CaCO3 saturation, budgets and fluxes of inorganic carbon, etc. As OrgAlk is associated with the presence of DOM and its organic acid-base species, areas receiving inputs of terrestrially derived or autochthonously produced DOM may exhibit an important contribution (i.e., organic alkalinity; OrgAlk) to the total alkalinity (TA). This fact is evident in the upper Arctic and tropical ocean zones, as well as in coastal areas.

104. Though we have the best practices for ocean acidification and OAE now, I am unsure how many actually follow this. Therefore, I am in fully support of this workshop. In addition, we can have **monthly online lectures/tutorials** to reach out a wider community.

(b) Suggestions specifically concerning mCDR

7. I think any practical skills (like using software or knowing how to use simple models) will be very important for this, both for students and mCDR.

16. Carbonate chemistry stands out to me as a major knowledge/skill gap at my career stage (students/postdocs, even some early faculty). I've interacted with lots of **folks who treat carbonate chemistry solvers as black boxes - without understanding how they work or which variables might matter for their calculations** - and unfortunately end up with a different result than they wanted.

This seems especially prominent and problematic in the growing mCDR field, where accurate carbonate chemistry calculations make a big difference.

19. …For mCDR, although the topic is widespread in the community and the number of ongoing projects is rising, lab experiment, mesocosm experiment, field experiment results are still in a shortage. It is very important to include researchers on these topics.

34. One of my major frustrations in the mCDR space is **connecting the expectations of monitoring and modeling for ocean alkalinity enhancement with the realities of what we can measure in the ocean and how we evaluate it**. We have capacity gaps in the number of labs that can rapidly analyze DIC/TA, limited consensus on what sensors work well in what environments, and labor and capital costs across this space aren't particularly well communicated. We see carbon registries and NGOs developing protocols and standards for carbon removal that miss many of these details or proscribe sampling and sensing at a level that is not yet commercially feasible. Educational tools across this space would simplify communication on the needs for funding for basic physical chemistry monitoring needs throughout mCDR projects.

38. mCDR is going to require a robust next generation of ocean carbonate chemists who can dig into the physical chemistry issues that come along with it. **We need that with or without mCDR, but the potential fast pace of the industry may accelerate the need at a time when we lack capacity.**

39. This call to arms is timely given the growing interest in carbonate chemistry by mCDR practitioners. There's a growing private industry that will be reliant on trustworthy and high precision carbonate chemistry measurements. The scientific community should play a large role in forming standard practices used in this emerging field.

When it comes to carbonate chemistry and mCDR, I don't know that there's necessarily a "skills gap", per se, e.g., it's not as if the community is forgetting how to do quality measurements. Rather, it seems like there's **more demand for chemical oceanographers with experience with carbonate chemistry than supply of trained experts**. The title of "chemical oceanographer" can get you a job as a lead oceanographer for a mCDR company even if your PhD is on a completely different subject like nutrient cycling. In this example, you have expert scientists learning a new sub-field and methodologies, so streamlining access to informational resources would be fantastic as these folks setup labs. **Interlab comparison studies and method sharing is also a good way to bring newcomers up to par with the gold standard labs**. If the mCDR industry is successful in the next 5-10 years, this will also represent a new pathway for oceanographic careers. We should prioritize getting new students trained on this topic and the underlying chemical methods.

42. I think this is fantastic, I keep seeing people working on mCDR that don't understand the physical chemistry and are oblivious to what should be obvious problems/challenges to experiment design and methods.

(c) Trace metals

51. **Metal cycling** and ocean mass balance (inputs/outputs)

59. My research interests include freshwater and terrestrial geochemistry, particularly the **speciation of trace metals and its consequences for fate and exposure to biota**. Speciation model

development and application is a key part of my research. As a late career researcher, I am facing issues in finding early career researchers in the UK with skills and interests in continuing these lines of research, which sounds rather similar to the issues that you are facing. So I would certainly agree that there are capacity building issues in relation to the physical chemistry of aqueous solutions and that these extend across the terrestrial and freshwater fields as well as in chemical oceanography.

60. **Nutrient & Trace metal speciation** & kinetics in climate scenarios.

74. **Trace metal organic speciation** - there are different competitive ligands, different considerations that should be addressed. On the other hand, we need more information about individual ligands and trace metal complexes and redox cycles.

84. A new global intercomparison study on **organic trace metal complexation** (especially Fe and Cu) in marine waters is urgently needed. There is no standard reference material for this type of study and the consolidation of complete analytical protocols is a prerequisite to obtain comparable data across different studies.

90. Gaps in **organic-metal-complexation**, no harmonization of methodology and practices across the field

95. I would like to draw attention to the extreme lack of research in the physical chemistry of **sediment pore water**. There is increasing attention to trace metal fluxes at the sediment-water interface, which play a major role in setting the whole ocean budgets of many trace elements. Yet the physical chemistry of pore water has rarely been studied, and many speciation models do not extend to pore water which is often distinct from seawater.

97. Since I am personally interested in **trace metal speciation in seawater**, I have realized we need more physical chemistry skills. I support to have the workshop which will improve our physical chemistry skills.

100. ..equilibrium dynamics of nutrient exchange in the interface of sediment and seawater in the bottom; transformation of organics reached from the sea surface to bottom, their role in nutrient recycling or exchange to the water.

(d) Kinetics

1. We don't just have to focus on the thermodynamics of marine chemistry. Looking at the open questions in **kinetics** would be good too.

17. Need **increased coverage and breadth in Kinetics. Physical Chemistry is more than Thermodynamics.**

37. skills gaps: **controls on speciation** and how to design sampling programs to constrain those controls

56. Kinetics setting the profile of observed trace metal and radio nuclides in the ocean (i.e. scavenging, aggregation, remineralisation etc.)

(e) Measurements and analytical techniques

14. I believe assumptions underpinning analytical techniques should be emphasized, specifically with regards to sample collection and voltammetric analysis. I also believe that internal (laboratory) consistency is the most impactful, however, laboratory inter-calibrations have proven to be immensely useful for construction of oceanic maps and consensus building.

58. (1) Experienced sea-going analysts for DO, nuts, carbonate chemistry, CFCs - vital for e.g. GO-SHIP, long-term changes, but also calibration of lowered and moored BGC sensors. Need experienced analysts to ensure any QC issues are picked up and remedied. (2) Available nutrient CRMs now much more akin to Pacific concentrations. (3) maybe not relevant, but also expertise and manpower in calibrating Argo-BGC measurements and BGC sensors on other autonomous platforms (which will become more prevalent).

80. Reliability of data and metrological aspects of measurements

92. **Instrumentation** is a key gap among scientists and practitioners.

93. Focus on training scientists in the **operation and interpretation of advanced analytical instruments** such as mass spectrometers, NMR spectroscopy, and X-ray diffraction.

• Conduct training in fieldwork methods, sample collection, preservation, and analysis to ensure high-quality data collection and interpretation.

(f) Modelling

4. Filling skills and knowledge gaps is essential to the field, but it is equally important that state-of-the-art aqueous chemical tools are made accessible for *correct* use by the wider community of non-experts. **The majority of current tools are opaque, sparsely documented, and require in-depth knowledge to use an apply.**

69. Methods of modelling coupling software technology and remote sensing technology

75. **Simple interactive models** that students can use to modelize future scenarios and their impact in different cycles (i.e. temperature, heat transfer, precipitation, salinity effect, trace metal distribution and speciation).

(g) Other areas

11. There is little time in introductory marine chemistry for a clear introduction to the thermodynamics of marine systems, let alone to kinetic processes in such a heterogenous environment. Furthermore, there are – I feel – no good textbooks that address these areas.

22. Skills/knowledge gaps: 1) **Ocean sediment + alkalinity interaction**; 2) Detailed understanding of **mineral surface processes controlling dissolution rates** (e.g., passivation, incongruent dissolution, atomic-level mechanisms, and related methods/engineering for overcoming kinetic barriers)

44. Need to include **thermodynamic parameters** in oceanographic applications to name a few: **pressure, enthalpy and heat capacity**.

57. The transfer of volatile amines from the sea to atmosphere is related to seawater pH. The presence of these molecule in the marine aerosol links their sea to air flux as a key source of base to the atmosphere and component of new marine particles.

93. Other recommended focus areas…
- Foster interdisciplinary communication and collaboration skills to facilitate integrated research approaches.
- Train on data science, statistical analysis, and database management.
- Training in remote sensing techniques, satellite data analysis, and interpretation to monitor ocean dynamics.
- Training in climate modeling, carbon cycle dynamics, and ocean acidification to assess and mitigate the effects of climate change on marine ecosystems.

100. a. thermodynamics, free energy, entropy, and related parameters relations against ocean chemistry. Many fewer studies regarding the entropy change in the last 100 years, so that scientists may explain well regarding the current climate change scenario.
b. **electrochemistry** of seawater not fully explored, for explaining seawater acidification and related aspects…

7. Research in less developed countries

The responses we received were from Central and South America, and from China. See also Appendix 2 for the perspective of a scientist from a western country working in China.

49. My research work is currently mostly in biological approaches on ocean acidification and alkalinization, I am in Ecuador where **equipment, consumables, reagents and infrastructure is quite limited**. Thus, my priority is to enhance my biological measurements, but still I need to have and improve my chem measurement. For many year I saw an increase in accuracy on measurements in sites where already exists a lot of information, while **most of the Equatorial and Tropical areas are neglected, not only for local limitations but because unachievable expectations from industrial high-income countries that act as deterrent for several scientists in developing countries to even try to measure**, because the quality of data will never be enough and publishable under those standards. On the other hand, we are still lacking data from most of planet surface. Thus, how to find the bridge to overcome the just high accuracy and frequency of measurements within an scope limited to high income countries' interest areas, and arrive to a sufficient geographical coverage as to have models that can represent more accurately the "grey" areas in maps by involving and supporting local scientist . Notice that many papers depict Equatorial information based in resolutions of about 200 sq km, and discuss and conclude based in so weak evidence.

50. As a scientist/professor in Latin America, one of a common problem observed is that the application of new knowledge and techniques can most of the time not be implemented due to the **lack of infrastructure and training**. However, local and regional funding agencies open calls to conduct these "hot research topics", resulting in a financial resource flow without significant/valid scientific outcomes.

98. The capacity building for physical chemistry should be exclusive for all people with different economic status for their countries or career stage. This is **especially important for those from least developed countries and early career scientist**. They should have equal opportunity to participate even the economy can be a constrain for conducting cutting-edge sciences.

8. Recommended networks and contacts

In this section are the responses to our second request "*Please share any ideas or feedback you have on networks or contacts we should engage in this community endeavor*." We first list those suggestions that include groups and networks, and in the second subsection those that include the names of individuals.

(a) Groups and networks

11. Scientific societies such as AGU, EGU, TOS, ACS, . . .

19. For standards and uncertainties, NIST people are great references. (NIST inorganic chemistry group: Jason Waters, Regina Easley, etc.)

For mCDR: private companies such as Ebbcarbon, Planetary. Dalhousie University working on the Halifax project. UMCES and UD working on the Chesapeake Bay project (my current group).

I am willing to get involved by representing Wei-Jun's lab at University of Delaware. We are currently working on the mCDR project with UMCES and Planetary. Previously, I had some connections and exploring experience on the organic alkalinity research. I have connections with the NIST group (Foreign Guest Researcher in the group mentioned above). And I had learning experience with Simon and David on the MarChemSpec model.

22. General idea: for CO2 mineralization, similar research seems to be progressing simultaneously in separate fields (geochemistry, mining/metallurgy, and cement). Some of the open questions in this topic are relevant to ocean chemistry (e.g., mineral precipitation, metals extraction/speciation). Expanding your focus across these subject areas may be useful to answer targeted questions. (...and also to progress geochemical CDR and decarbonization efforts more broadly.)

26. Maybe the community of GEOTRACES

27. See who is chairing the Environmental Sciences:Water Gordon Conference and perhaps they will promote this. Also look at session chairs at Goldschmidt.

32. Not sure of networks. One comment: I've been recruiting undergraduates with degrees in chemistry and chemical/environment engineering

34. It would be interesting to connect with the enhanced rock weathering folks on this space. I'll pass the original email around. It could be useful to post this on the CDR google group (https://groups.google.com/g/CarbonDioxideRemoval) and other listservs (news@carbondioxide-removal.eu). It would be useful to send this directly to NIST (Pamela Chu) as well, as they have interests in standards development.

36. Regina Easley and Jason Waters at NIST. For the younger community, there is a group called GOA-ON ICONEC (International Carbon Ocean Network for Early Careers) that could draw significant interest.

38. National institutes of standards and technology, the next gen (graduate students, postdocs, ECRs)

39. Ocean Visions has a nice map showing who in the world is doing mCDR work. Most institutions on that map would probably be interested: https://oceanvisions.org/mcdr-field-trials/mcdr-field-trial-map/

45. REMARCO (https://remarco.org)

49. GOA-ON, Remarco

51. Involve mentoring groups and organizations that support diversity in the field, such as GeoLatinas

52. Other SAMS researchers have contacted you e.g., Robyn Tuerena MASTS biogeochemistry forum.

53. Certainly the Global Ocean Acidification - Observing Network. Helen Findlay (hefi@pml.ac.uk) is in the Executive Council and chairs the North East Atlantic hub and the mCDR working group

54. National Chemistry foundations/professional networks, e.g. Royal Society of Chemistry in UK

55. From a metrology perspective, perhaps invite entities like NIST and UK LGC?

56. GEOTRACES

57. Professor Rafel Simo and colleagues at ISM, CSIC, Barcelona (rsimo@icm.csic.es)

60. Biosensors & microbial Bioavailability

61. GEOTRACES, BIOGEOSCAPES

63. Engaging Chemistry-oriented networks (i.e., RSC)?

66. Geotraces community; SOLAS; SCOR,

67. I contacted people from GEOTRACES in Spain

69. You are well connected as far as i know.

72. Any international bodies like IOCCP, GEOTRACES, GOA-ON or IAPSO, but also metrology coordination institutions like BIPM and CIPM.

74. GEOTRACES, BIOGEOTRACES

75. GEOTRACES, and probably contact with Toby Tyrrell (with his "simple" models he uses in his course).

76. Mediterranean Ocean Acidification Hub, OA Med-Hub Voluntary Commitment, Network and contacts: Dr. Abed El Rahman Hassoun, ahassoun@geomar.de, abedhassoun@cnrs.edu.lb; http://www.goa-on.org/regional_hubs/mediterranean/about/introduction.php

Pier2Peer network and contacts: elise.keister@noaa.gov or Alexis Valauri-Orton and Kaitlyn Lowder at IOAI@oceanfdn.org; http://www.goa-on.org/pier2peer/pier2peer.php

85. Geotraces, Biogeoscapes and mCDR communities

92. Chemical hydrologists, Chemists, and Environmental scientists from developing countries.

93. Researchers at the Kenya Marine and Fisheries Research Institute

94. Without the support of funding agencies it would be very difficult to promote capacity building in physical chemistry of seawater. Funding is a major concern as physical chemists in many countries do not seem to be able to get large or long-term support. Even for a guru like Frank Millero he had to venture into measuring carbonate parameters in the oceans to get major funding to supplement his love of the physical chemistry of seawater.

95. I would recommend to build better connections between oceanographers who study the water-column with those who study sediments. Also it would be great to create community reports on the best practices of ocean chemical modeling.

97. The workshop will be helpful especially for early-career ocean scientists.

98. The community should get in touch with UN Ocean Decade through Decade Advisory Board, Strategic Communication Group, programme and project. The UN Decade is a great platform for getting everyone involved in science as well as policy making. This can be helpful for the scientist from least developed countries to get involved in the carbon cycle and ocean studies. The Decade advisory board can be reached though any of the committee members (https://oceandecade.org/decade-advisory-board/). And I can be contact for Strategic Communication Group (yuntao.wang@sio.org.cn).

104. There are many early career networks (e.g., SOLAS, IAPSO, IIOE-2, IMBER, EGU) that must be targeted. They have official webpages. In case you are unable to reach, I can help with it.

(b) Individual contacts

13. I sailed with Will Berelson (USC), Jaclyn Pittman Cetiner (USC), and Jess Adkins (Caltech/Calcarea) on a cruise focused on in situ CaCO3 dissolution in sediment. The USF lab was tasked with measuring pH and AT, but other CO2 system parameters, like CT and C-isotopes, were also measured. Most seem to be transitioning towards mCDR or OAE, but they could be good, reputable contacts if we want to expand our network into that field.

24. Dr. Robert Byrne, Dr. Xuewu Liu

52. Other SAMS researchers have contacted you e.g., Robyn Tuerena MASTS biogeochemistry forum.

57. Professor Rafel Simo and colleagues at ISM, CSIC, Barcelona (rsimo@icm.csic.es)

59. I can provide some names of freshwater/terrestrial researchers with similar skills/interests to myself in Europe, who may be interested in this initiative:

Prof Marc Benedetti (benedetti@ipgp.fr)

Prof Jon-Petter Gustafsson (jon-petter.gustafsson@slu.se)

Dr. Jan E. Groenenberg (bertjan.groenenberg@wur.nl)

Dr. Remi Marsac (remi.marsac@univ-rennes1.fr)

62. I've forwarded this on to my former postdoc, Ross Whiteford, who led a recent paper (in revision) on this topic, along with Oscar Branson, who collaborated on it. Matthis Hain at UCSB has also been working on this topic and would be good to have involved.

75. GEOTRACES, and probably contact with Toby Tyrrell (with his "simple" models he uses in his course).

76. Mediterranean Ocean Acidification Hub, OA Med-Hub Voluntary Commitment, Network and contacts: Dr. Abed El Rahman Hassoun, ahassoun@geomar.de, abedhassoun@cnrs.edu.lb; http://www.goa-on.org/regional_hubs/mediterranean/about/introduction.php

Pier2Peer network and contacts: elise.keister@noaa.gov or Alexis Valauri-Orton and Kaitlyn Lowder at IOAI@oceanfdn.org; http://www.goa-on.org/pier2peer/pier2peer.php

79. joelle.salaun@shom.fr

80. Florence Salvetat (IFREMER) Florence.Salvetat@ifremer.fr

91. Dr. Pavel Tishchenko, Leading Researcher at Pacific Oceanological Institution, Vladivostok, Russia

Appendix 1. Our solicitation to the oceanography community

The copy of our solicitation for responses, below, summarises what we see as the significant and growing problem in the field of chemical oceanography and its applications. It proposes a workshop as the first step towards addressing this, and states its aims.

Building Capacity in Physical Chemistry Methods, Measurements and Modelling for Chemical Oceanography

The fundamental physical chemistry of natural waters, e.g., acid-base speciation, trace metal complexation, and mineral solubility, is central to chemical oceanographic problems such as:

- Resolving uncertainties and inconsistencies in the relationships of the parameters of the marine carbonate system.
- Developing calibrations and standards for pH and other quantities.
- Understanding the relationship between atmospheric CO_2 and the carbonate and silicate cycles in past oceans, which have different compositions from the present day (paleoceanography).
- Marine carbon dioxide removal (mCDR), in particular the effects of electrochemical methods and mineral additions close to the areas of application where seawater composition and chemistry may be disturbed from normal values.
- The biological availability and fate of trace metals (complexed by inorganic and organic seawater components).

The above are examples related to our own work, and are not exclusive. Many of these and other applications are relevant not just to the oceans, which have a largely invariant composition with respect to major inorganic components, but also to enclosed seas, estuaries, and pore waters, which have different compositions and a different physical chemistry.

We are concerned about dwindling expertise in the physical chemistry of aqueous solutions that is so foundational to the field of chemical oceanography. We are writing to you in order to gauge the level of interest and solicit ideas from the oceanography community to catalyze capacity building and continued research in this area. This, we believe, should begin with an international workshop to bring together chemical oceanographers across sub-disciplines and applications with leading scientists from other fields with relevant expertise (e.g., other areas of geochemistry, chemical engineering, etc.). It would aim to:

1. **Assess the science**: Share knowledge of experimental methods and modeling tools and theory, and highlight opportunities for community-wide activities (intercomparison, synthesis, development of best practices, etc.) that can make the best use of our current capabilities.

2. **Identify opportunities**: Determine the subject areas within chemical oceanography that are impacted by the lack of physical chemistry skills in both modeling and experimental methods, and what is needed to address this skills gap including, for example, strengthening collaborations with scientists in other disciplines.

3. **Support the next generation:** Strategize curricular, training, and capacity building mechanisms to increase and then maintain the skills and expertise required to carry this field forward.

4. **Build community:** Explore ways of developing a more cohesive and collaborative network of aqueous geochemistry practitioners working in the field of chemical oceanography.

During the 2024 Ocean Sciences Meeting, we initiated discussions with national funding agencies and various oceanographic organizations and networks regarding the concerns and ideas laid out here. There is recognition that we have identified a real problem. **To be successful, the workshop needs to foster discussions, planning, and knowledge transfer across career stages and disciplines, especially with those outside the field of oceanography. It also needs to develop clear recommendations.** We are willing to spearhead a workshop proposal and lead such an activity, with the intention that it will strengthen our community and, particularly, generate new initiatives in training and research in physical chemistry measurements and models for applications in oceanography. We would aim for such a workshop to take place in late 2024 or early 2025.

How can you get involved?

Community support is critical for securing funding for this activity and its outcomes. **To express your interest in a potential workshop and provide feedback on ideas summarized here, please either email one of us or CLICK HERE** (https://forms.gle/ztqhatTZXLU8tW8p6). Even short comments outlining your needs and experience will be valuable and will help shape a proposal.

Please share this document with colleagues you think might be interested.

Thank you for your time,

Heather Benway (Ocean Carbon & Biogeochemistry Project Office, Woods Hole Oceanographic Inst.), hbenway@whoi.edu

Simon Clegg (Joint Committee on the Properties of Seawater, Task Group on Chemical Speciation, Univ. East Anglia), s.clegg@uea.ac.uk

Appendix 2. Comments received on likely interest from Southeast Asia

Below are comments received on likely interest from Southeast Asia, from a scientist (a UK national) who works at a university in China:

> I would generally agree that some of these topics, particularly mCDR are 'sloppy', at best when it comes to a firm grasp on the basic underlying concepts, and it would be useful to think about what the actual problem is there - probably not lack of knowledge but perhaps a more messy situation related to how this work is promoted/funded and the conflicts of interest there.
>
> But I think perhaps the perception of a 'developing skills gap' is a very N American/W Europe one. I think it's worth remembering that the majority of the world's scientists live in a circle centered on SE Asia, they aren't well represented -if at all- at American conferences or in US/European led 'international' programs, and largely make their own networks which aren't US centered. In China, marine chemistry was not until very recently a major focus with 'ocean science' previously being largely geophysics, but I think physical chemistry is now quite well represented, growing quickly as a field, and there are plenty of people working on it. My perception here would be that skills gaps in physical chemistry are closing very quickly rather than opening. I'm not sure there would be much interest in many of these groups joining 'international' workshops as I think the experience of my colleagues in China and more broadly SE Asia is 'international' programs usually under-represent them and are almost universally perceived, whether justifiably or not, as not making serious efforts to engage the none-N American/W Europe scientists.
>
> This issue particularly affects international standards, protocols etc because these are often drawn up by groups of scientists who overlook the issues faced working outside the US/Europe, e.g. is the equipment referred to physically available in other countries, can standards physically be imported, are the guides/recommendations/protocols etc compatible with how research has been done for many decades worldwide or only within a specific group. To give the last example I can think of, I recently read an OAE 'best practice guide' which was designed to guide OAE development globally, the authors based their recommendations on all the work they were aware of which was explicitly stated to be German/Belgian/US, but there are very longstanding OAE programs in Malaysia and extensive work in China, India, Spain and Italy that the authors were presumably not even aware of. So the perception in some circles will unfortunately be that a group of western experts has written a 'global' guide which they presumably expect to be used, without making many efforts to be aware of the global situation.
>
> Xiamen, Shenzhen, Guangzhou and to a lesser extent Shanghai have growing marine chemistry communities, but I think to be honest they will be luke-warm about anything like this, they are regularly asked to engage with US/EU led projects but there just isn't much interest in that here. I think the way they see it is that there are already well-established networks here which 'outsiders' completely ignore. If you want to make some progress, someone might want to do a session at XMAS, the closest thing there is to an Asian Ocean Sciences, their call for sessions for the 2026 conference is open, it's got a very healthy marine chemistry content.

Appendix 3. Programmatic Letters of Support

Below are letters from SOLAS and from GEOTRACES.

SOLAS International Project
Offices State Key Laboratory of Marine Environmental Science, Xiamen University, China
National University of Ireland Galway, Ireland
solas@xmu.edu.cn

25 July 2024

Dr. Heather Benway, Woods Hole Oceanographic Institution, MA, USA
Dr. Simon Clegg, University of East Anglia, UK

Subject: SOLAS Support for the workshop on "Building Capacity in Physical Chemistry Methods, Measurements and Modelling for Chemical Oceanography

Dear Drs. Benway and Clegg,

With this letter SOLAS expresses its strong support for the development and planning of an international workshop on "Building Capacity in Physical Chemistry Methods, Measurements and Modelling for Chemical Oceanography."

We are happy to learn of the enthusiastic response from the oceanographic community in pushing forward with this workshop. SOLAS has a long history of linking the physics and chemistry of processes that control air-sea exchange and, accordingly, also recognizes the great importance of building on the legacy of current quantitative physical chemical models. This activity is critical for continued progress in unraveling atmospheric and marine chemical processes that form the fundamental tapestry on which biogeochemical cycles operate. SOLAS is currently developing its next Science Plan (2025-2030) which includes major initiatives directed at "science for solutions" and "capacity building." We are dedicated to develop the scientific capacity that will contribute the ocean-atmosphere expertise needed to address some of the grand challenges in earth systems with well-considered action.

With its emphasis on physical chemistry, the goals this workshop plans to address are highly relevant to SOLAS priorities, particularly those related to foundational carbonate chemistry, metal chemistry and bioavailability, as well as the opportunities developing around mCDR. Planned outcomes for this workshop in the physical-chemical community (identifying opportunities, strengthening collaborations, expanding expertise, supporting the next generation) are well-matched to, and compatible with foundational SOLAS goals for the air-sea community. We see important overlap and hope this develops into an area of productive cooperation.

Best of luck in pursuing this important event and please keep SOLAS abreast of developments.

With very best regards,

Dr. Christa Marandino
Co-Chair, SOLAS Scientific Steering Committee

Dr. William L. Miller
Co-Chair, SOLAS Scientific Steering Committee

Dr. Li Li
Executive Director
SOLAS International Project Office

GEOTRACES

An International Study of the Marine Biogeochemical Cycles of Trace Elements and their Isotopes

8 August 2024

Heather Benway
Ocean Carbon & Biogeochemistry Project Office
Woods Hole Oceanographic Inst., Woods Hole, USA

Simon Clegg
Joint Committee on the Properties of Seawater
Task Group on Chemical Speciation, Univ. East Anglia, Norwich, UK

Reference: International workshop "Building Capacity in Physical Chemistry Methods, Measurements and Modelling for Chemical Oceanography"

Dear Heather and Simon,

We are writing in our capacity as co-chairs of the international GEOTRACES program to express our support to the organization of an international workshop to build capacity in physical chemistry methods, measurements and modelling for chemical oceanography.

GEOTRACES (www.geotraces.org) is an international research program dedicated to understanding the marine biogeochemical cycles of trace elements and their isotopes. For more than a decade, GEOTRACES has brought together scientists from over 35 countries to map the distribution of trace elements and their isotopes in the global ocean and understand the processes regulating their distribution.

As co-chairs of an international marine geochemistry program, we recognize the need to generate new training and research initiatives in the field of physical chemistry measurements and models for applications in oceanography and share our concern about the diminishing expertise in this boundary area between physical and marine chemistry, which underpins the field of chemical oceanography. It is essential to organize an international workshop that generates international interest in this field and creates and strengthens a community of oceanographers across sub-disciplines and other fields with relevant expertise, capable of catalyzing these new initiatives. We therefore fully support this proposal for an international workshop.

Yours sincerely,

Prof. Karen Casciotti
kcasciot@stanford.edu

Prof. Jun Nishioka
nishioka@lowtem.hokudai.ac.jp

Prof. Alessandro Tagliabue
A.Tagliabue@liverpool.ac.uk