OH, ceriously, ... Molecules + materials = difficult!

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Materials and their surfaces and interfaces play crucial roles in our society and in the development of new technologies. Modelling such complex systems is by no means easy, and the computational scientist needs to make shrewd decisions about both (i) how to build *a structural model* that captures the complexity and imperfections of the real system at hand, and (ii) how to find an interaction model (say a DFT functional or a force-field) that is good enough. In particular, in this talk I will elaborate on the following topics with examples from water/solid interfaces, molecular crystals and metal oxide nanoparticles.

1. *Can we capture the chemistry of redox-active systems without including the electrons?*

   In the quest to reach larger and more complex systems sacrifices have to be made. Redox-active materials (with d and f elements) constitute a challenge for DFT calculations and force-field simulations alike and combining them in a *multiscale modelling* protocols is no easier! Is it possible to achieve a seamless linkage? Is it even possible to capture some chemistry without the electrons? Combinations of DFT, tight-binding-DFT, and reactive force-field models will be presented (see e.g. [1]). **Ceria** (CeO_2) is an example.

2. *Computational spectroscopy – as good as experiment?*

   Modelling is now an indispensable tool to decipher and interpret spectra and images produced from experiments, and adequate models for *post-processing* is as important as the data generation itself. I will discuss vibrational spectra in the context of AIMD simulations neural-network generated potentials and force-fields. **OH** groups, i.e. water and hydroxides, at solid/liquid interfaces [2] will be one example.

3. *How accurate are DFT methods for complex materials*?

   For condensed-matter systems of some complexity, there exists no quantum-mechanical or other theoretical method accurate enough to serve as a golden standard, so access to good-quality experimental data is crucial. Complex crystals can be promising benchmark systems as there often exist experimental structural data, the atoms stay put, and a large range of structural motifs is represented. [3]

I will also inform about the European Materials Modelling Council (https://emmc.info/), and our efforts to promote the use of materials modelling in industry and increase the trust in modelling results, and our efforts to seek a balance between physics-based and data-driven approaches.

References

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3. G. G. Kebede, P. D. Mitev, P. Broqvist, J. Kullgren, and K. Hermansson, **2018**, *J. Phys. Chem.* **C 122** (2018) 4849.