Developing Software for Your PhD Research

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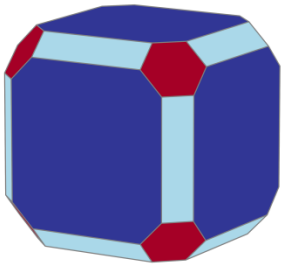
High performance simulation software is at the heart of computational chemistry and is used to answer a wide range of research questions. These simulations rarely yield a “publication ready answer” and significant data analysis is needed before the data yields useful information. While this data analysis is usually performed in isolation, a significant number of analysis codes are published (1), allowing the spread of ideas, improvement of software and increased collaboration. One such code, surfinpy (2), has recently been published in the journal of open source software and analyses surface adsorption data generated from any energy minimisation calculation. surfinpy generates surface phase diagrams, calculates desorption temperatures and determines particle morphologies. In this talk I will outline the software development and publication process before discussing an example of surfinpy being applied to the adsorption of water on doped cerium oxide surfaces. I will discuss the full workflow that ranges from the calculation of simple adsorption energies to predicted particle morphologies and apply this analysis to soot oxidation catalysts, water gas shift reaction catalysts and nanoparticle aging.

Keywords – Python, Open source software, Cerium Oxide, Nanoparticles, Catalysis, Water adsorption.



How does water adsorption affect the particle morphology of Cerium oxide?

(1) - https://joss.theoj.org/

(2) - AR. Symington, J. Tse., M. Molinari, A Marmier and SC. Parker *Journal of Open Source Software* **2019**, *4*, 1210