Modelling olivine surface properties: assessment of methods and tools.

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The ability to build realistic models of the main crystal surfaces of olivines is crucial to investigate the fundamental interactions responsible for the wide range of chemical and physical processes occurring at the olivine interface.

Due to the complexity of these processes, which include nucleation and dissolution, electron transfer, physical and chemical adsorption, the development of both force field and ab initio models is extremely important. In the last few years, a few papers takling the complex task of developing quantum-mechanical [1-3] and classical [4-6] models have appeared, though a critical assessment of their performance has never been undertaken. On top of this, the main surfaces of olivine have been fully considered only with force field models, and only for the Mg end member (forsterite).[4,5]

We present here an accurate ab initio study of the structure and surface energy of the (010), (101), (111), (001), (110), (120) and (021) surfaces of forsterite.[7] The ability of some of the most widely adopted DFT schemes to address this task is discussed. Gaussian type basis sets of different quality have been considered, including those recently developed by Peintinger *et al*. [8] allowing to perform solid state calculation at a TZVP level.

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