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Structural and vibrational properties of sulphate-water clusters from ab-initio calculations QUAN WAN, LEONARDO SPANU, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis — Hydrated clusters of sulfuric acid derivatives play an important role in many processes of interest, e.g. environmental sciences and electrochemistry. Determining their structural and electronic properties is a challenging task: they exhibit a complex free energy landscape and there is no direct experimental measurement of their geometry, which is usually inferred from spectral signatures obtained, e.g. by infrared (IR) measurements [1]. We have used *ab initio* molecular dynamics simulations to investigate the stability, electronic properties and IR of sulphate-water clusters containing 12 and 13 water molecules. We discuss how the entire hydrogen bonded network of the cluster may be affected by the presence of a single, additional water molecule, leading to geometrical arrangements not yet identified in experiments. We also show that clusters with different structures may have similar IR spectra, thus making it difficult to use spectral signatures to unequivocally determine the cluster geometry. Finally we discuss the electronic properties of the clusters and in particular differences obtained in the computed ionization potentials when using semi-local and hybrid functionals.

[1] Zhou *et al.* J. Chem. Phys. **11,** 111102 (2006)).

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