Two-dimensional silica - Defects, adsorption and vibrational properties

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The recent finding of a 2-dimensional (2D) SiO2 bilayer structure has recently attracted attention, both for being a stable 2D compound and for its existing in amorphous forms as a 2D glass[1–3]. By combining first-principles and classical force field calculations with aberration-corrected high-resolution transmission electron microscopy experi- ments, we study the morphology and energetics of point and extended defects in hexagonal bilayer silica (HBS) and make comparison to graphene, another 2D system with a honeycomb lattice. We show that the motifs of isolated point defects in these 2D structures with otherwise very different properties are similar, and that the morphology and energetics of extended defects, such as grain boundaries have much in common as well[4]. The vibrational properties of HBS are studied by calculation of the phonon spectrum. We show how the easily compressable HBS lattice is at equilibrium situated at a structural phase transition, which makes calculation of phonons particularly challenging. We demonstrate that the calculated spectrum compares well with experimental data from Raman and infrared spec- troscopies. Furthermore, the binding to different metal surfaces of HBS and its epitaxial sibling, hexagonal monolayer silica are studied by means of first-principles calculations to shed light of the growth process of 2D silica polymorphs.[5]

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[3] Lichtenstein et al., *Angewandte Chemie International Edition* **51**, 404 (2012).
[4] Björkman eta al., *Scientific Reports* **3**, 3482 (2013).
[5] Ben Romdhane et al., *ACS Nano* **7**, 5175 (2013).