Adsorption and defects of 2-dimensional silica

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The recent finding of a 2-dimensional (2D) SiO_2 bilayer structure has recently attracted attention, both for being a stable 2D compound and for its existing in amorphous forms as a 2D glass[1,2]. In the present study, we investigate the binding to different metal surfaces by non-local correlation functionals, a sophisticated density functional theoretical method that properly accounts for van der Waals interactions[3]. Furthermore, we study the formation energy of defects similar to those that appear in graphene, another honeycomb lattice, and which have also been found experimentally in pristine 2D SiO_2. The results show large qualitative similarities with the defect structures in graphene, but also quantitative differences that arise from the differences in the binding structure compared with graphene. The strain fields around the defects are studied and found to be exceptionally long ranged, a serious practical problem which is overcome by a careful compari son of results obtained with classical potentials with first-principles data. We also study so-called Haeckelite structures, hypothetical structures obtained by periodically reproducing the defect throughout the lattice. When allowing for full relaxation of the structure, the total energies of the Haeckelite structures exceed those of the ideal honeycomb lattice by surprisingly small amount, showing that formation of amorphous structures should indeed be expected.

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[2] L. Lichtenstein et al., *Angewandte Chemie International Edition* **51**, 404 (2012).
[3] T. Björkman, *Physical Review B* **86**, 165109 (2012).