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First principle study of SiO_2 bilayer on metallic substrates[1] XIN LIANG, Department of Applied Physics, Yale University, ANDREI MALASHEVICH, SOHRAB ISMAIL-BEIGI, Center for Research on Interface Structures and Phenomena and Department of Applied Physics, Yale University, ERIC I. ALTMAN, Center for Research on Interface Structures and Phenomena and Department of Chemical Environmental Engineering, Yale University — Silicates in zeolite form have wide applications in catalysis: they have porous structures with large internal surface areas. However, it is hard to characterize such internal surfaces with atomic resolution experimentally. Therefore, a 2D form of silica provides an interesting model system that can be probed using real-space methods such as scanning tunneling microscopy (STM). In fact, 2D SiO_2 bilayers can be created experimentally. Both crystalline and amorphous bilayers have been grown on various metallic substrates. Due to the fully saturated nature of the Si-O bonds, it has been argued that the SiO_2 bilayer and substrate interact weakly: however, the substrates can enforce epitaxial strain on the bilayer. In this work, we investigate to what extent metallic substrates (e.g. Ru and Pd) affect the stable morphologies of SiO_2 bilayers by using *ab initio* density functional theory (DFT). We are particularly interested in seeing how strain in the bilayer competes with substrate interactions and the nature of the resulting bilayer structures. This work is supported by the National Science Foundation through grant NSF DMR-1506800.

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