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The Nature of Metal-Oxygen Bonding at Corundum (0001) Surfaces in the Presence of Oxygen EMILY JARVIS[1], ORKID COSKUNER, ANNE CHAKA, National Institute of Standards and Technology, Physical and Chemical Properties Division, Computational Chemistry Group — Metal oxides are of critical importance in a variety of applications ranging from gas sensing to catalysis to environmental containment of heavy metals. In all of these cases, it is the surface chemistry that is essential to the necessary function. The detailed surface structure is heavily dependent on the physical and chemical features of the surroundings, and its reactivity is largely dictated by the nature of the local bonding character. We use all electron density functional calculations combined with *ab initio* thermodynamic predictions to explore surfaces of several corundum-structured metal oxides as a function of oxygen partial pressure, which is a crucial first step in understanding corrosion, passivation, and catalysis. Additionally, we apply quantum mechanical wavefunction-based methods with the goal of elucidating the local bonding character of these surfaces. Our calculations provide detailed insight into the nature of the chemical bonding at chromia and hematite (0001) surfaces with M=O termination, i.e., the chromyl- and ferryl-terminated surfaces, and explain the dissimilar thermodynamic predictions for the alumina (0001) surface relative to these transition metal oxide surfaces.

[1]Membership Pending

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