Analysis of (110) and (113) corundum (α–Al_2O_3) – water interfaces from DFT–MD simulations

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Aluminum oxide and hydroxide minerals are abundant in the environments and are used extensively in technological applications. Consequently, the interaction between water and surfaces of the various alumina phases is of considerably interest. Despite numerous studies of alumina phases, particularly corundum (α–Al_2O_3), a detailed description of alumina–water interfaces is still incomplete. The relatively high solubility of aluminum oxide and hydroxide complicates the experimental approaches typically used to investigate mineral–water interfaces, resulting in many questions remaining unanswered. Molecular simulation studies have been used to gain a better understanding of corundum–water interfaces; however, studies have focused on the most stable basal (001) plane and to a lesser extent on the (012) surface.

The work presented here focuses on the (110) and (113) α–Al_2O_3 surfaces. Specifically, molecular-level detail of the (110) and (113) α–Al_2O_3 – water interfaces was obtained from DFT–MD simulations. Comparable simulations of the (001) and (012) – water interfaces were also completed. The Vienna *ab initio* simulation package (VASP)[1] was used for all calculations, which were completed at the same level of theory. The interaction of water molecules with surface atoms, the distribution of water dipoles, and H-bonding properties were analyzed for each surface. Atomic charges (Bader charges) at the surfaces, atomic density profiles of the surface structure and H-bonding were computed and compared. Additionally, vibrational density of states were calculated and interpreted. Finally, the molecular-level behavior of the four α–Al_2O_3 – water interfaces were compared, and variations were interpreted relative to the specific surface structure of the surfaces.

[1] Kresse, G. & Hafner, J. (1993) Phys. Rev. B, 48, 13115.