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First principles study of water adsorption on the (100) surface of zircon: Implications for zircon dissolution

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ABSTRACT

We have studied the interaction of aqueous species with the (100) face of zircon using first-principles quantum mechanical calculations. Adsorption energy of molecular water on the Zr Lewis site is 1.27 eV per molecule, whereas the energy of dissociative adsorption is only 0.84 eV per molecule. Thus, the non-dissociative adsorption of water is strongly preferred with respect to the dissociative adsorption on the (100) face of zircon. Such behavior, which is related to the weak ability of the surface structure to relax, is changed by a 5% increase of the surface cell parameters. From our theoretical results, we propose that the exceptional resistance of zircon to dissolution may be related to the strong acidity of the Zr-O-Si bridging O atoms, which promotes the associative adsorption of water on the (100) surface of zircon.