A molecular orbital study for the weathering mechanism of silica by acids

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The reactions between silica and some acids were studied by the molecular orbital method, in order to investigate the weathering mechanism in atomic scale. A silica surface is modeled by H_4SiO_4 molecule and four acids (H_2CO_3, HNO_3, H_2SO_4 and H_3PO_4) are applied to the silica molecule. The strategy to approach each acid to the silica molecule is employed ; the distance between H_4SiO_4 and each acid is changed and all the atomic coordinates are optimized to have the minimum energy at each distance. The Gaussian 94 program was used for the Hartree-Fock type molecular orbital calculations under the STO-3G basis.

The carbonic acid donates a hydrogen to a hydroxide (OH) of H_4SiO_4 to make a water molecule, the water molecule is emitted from the silica breaking the Si-O bond and instead, an oxygen of carbonic acid is bonded to Si atom. The atomic configuration has the total energy as low as the two independent molecules, indicating the possibility of the reaction. The nitric acid captures a hydroxide from H_4SiO_4 molecule and another oxygen of H_2NO_3 is bonded both to Si and N. Finally two oxygens of nitric acid are bonded to Si of H_4SiO_4 to be five-coordinated. The total energy is much lower than in the independent two molecules suggesting the high possibility of the reaction. Other two acids of sulfuric acid and phosphoric acid take essentially no role in the reaction.