

Abstract Submitted
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Monitoring bonding reconstruction across the α -cristobalite \rightarrow stishovite phase transition in silica ÁNGEL MORALES GARCÍA, Departamento de Química-Física I, Universidad Complutense de Madrid, Madrid, Spain, MIGUEL A. SALVADÓ, PILAR PERTIERRA, J.M. MENÉNDEZ, J.M. RECIO, Departamento de Química Física y Analítica, Universidad Oviedo, Oviedo, Spain, MALTA CONSOLIDER TEAM — We propose a microscopic mechanism that describes how the structure and bonding network of α -cristobalite transforms into stishovite at constant pressure and temperature. A martensitic-like approach that preserves the translational symmetry is used to modelize the simultaneous and coordinated movement of all the atoms as the transition progresses. Relevant distances and angles, cell strains, and atomic displacements across the transition path are obtained from first-principles calculations under the generalized gradient approximation of the density functional theory. A soft and symmetric energetic profile is computed with an activation barrier lower than 100 kJ/mol at the thermodynamic transition pressure. Thanks to the analysis of the calculated topology of the electron localization function, we are able to provide visual and quantitative information on the chemical bonding reorganization that accompanies this transformation, mainly the increasing of Si and O coordinations from 4-fold to 6-fold and from 2-fold to 3-fold, respectively. We do not detect any bond breaking, but the formation of two new Si-O chemical bonds involving oxygen atoms from the third coordination sphere of Si. It is not until the Si-O distance is close to 2.0 Å when the new bonds emerge.

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