High Pressure-High Temperature Reactions of CO_2 – SiO_2 systems

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Carbon dioxide and silicon dioxide, both group IV oxides, are two of the fundamental components in the Universe. Under pressure and high temperature, CO_2 is a supercritical solvent and, therefore, ivery likely that under the Earth's mantle conditions, may react with silica (SiO_2). The new compounds formed may play an important role in volcanic and seismic activityThe mineral This possibility has driven recent experimental investigationss on potential reaction between CO_2 and SiO. A disordered silicon carbonate was found from the compression of a mircroporous SSZ-567 zeolite filled with CO_2 at 18-26 GPa and 600-980 K. More inteerestingly, a crystalline cristobalite-type CO_2.SiO_2 solid solution was obtained from the reaction of CO_2 and molten silica at 16-22 GPa at 4000 K. Here we present results of First-principle density functional-based molecular dynamics (MD) and total energy calculations to study the reaction mechanisms, structures and propducts of the reactons of CO_2 with SSZ-567, molten silica and stishovite under high pressure and high temperature. The calculations reproduced the different products observeed by experiments. In addition, it provides detailed imechanistic information on the novel chemcial reactions and the physical and electronic properties of the products.

[1] Santoro, *et.al.,* (2011*). Proc Natl Acad Sci* U S A **10**8, 7689-7692. [2]. Santoro M, *et al*. (2014). *Nat Commun* **5**, 3761.