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High-temperature, high-pressure reactions of H_2 with $CaCO_3$ melts

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First-principles molecular dynamics calculations have been performed to investigate the reactions of hydrogen and calcium carbonate melts at pressure-temperature conditions appropriate to the Earth's lower mantle and core-mantle boundary. Two models with different hydrogen to carbonate ratios were studied. A variety of chemical reactions were observed. It is found that the hydrogen dissociated readily and reacted with free carbonate anions forming various transient chemical species and water molecules. Further reactions of these reactive species serve as intermediates to form C-C and C-O connections. The unreacted bulk carbonates are linked *via* polymeric cornered shared CO_4 tetrahedra. At 110 GPa and 4087 K “diamondoids” with tetrahedral C_4 moieties were found. The theoretical results support recent reports on the observation of tetrahedra CO_4 in high-pressure carbonate glasses and suggest a plausible explanation of ice VII inclusion in deep Earth diamonds.

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