The properties of $(Mg,Fe)CO_3$ in the earth mantle conditions

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The global carbon cycle has attracted the attention of scientists from a wide range of disciplines. Previous investigations have focused primarily on the atmosphere, oceans, and shallow crustal environments, but on long time scales, it is also affected by subduction and magmatism. Subduction carries carbon-bearing minerals down to mantle and magmatism releases carbon into atmosphere. Carbonates are a possible carbon host mineral in the Earth's mantle. If it is not stable or decomposes in the Earth mantle conditions, carbon transfer from surface to mantle will be limited. Therefore, it's critical to understand the stability of carbonate minerals at high pressure and temperature conditions. There have been many experimental [1, 2, 3, 4] and theoretical studies [5, 6] of $MgCO_3$ and $FeCO_3$ carbonates, but there is still much debate about their high-pressure structure. Here, we use first principle calculations to investigate these candidate structures in order to determine which best matches available experimental data**.** Our results should help to constrain the structure and properties of $MgCO_3$ and $FeCO_3$ at high pressure and temperature, providing insight into the possible role of the deep Earth in the carbon cycle.

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