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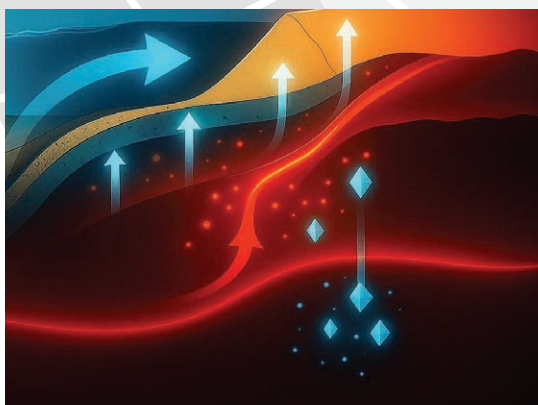
## Venue: Meeting Room #486

Science Research Bldg. 1, 4th floor.

Ehime Univ.

### Keywords

1. Deep carbon cycle
2. High-pressure phase transition
3. First principles calculations



# A new insight into the fate of subducted carbonates

The greenhouse effect of carbon dioxide has maintained a warm surface environment on the Earth over geological time scales. On the other hand, it is believed that atmospheric carbon dioxide concentration has steadily declined. This suggests that although most carbon fixed to organic materials through photosynthesis of phytoplankton and plants returns to the atmosphere, some fractions are stabilized as carbonate minerals, fossil fuels, etc. and sequestered from the biospheric environment, and a portion is further sink down into the Earth's interior along subducting oceanic crust. Although most of subducted carbon are also thought to return to the atmosphere via degassing reactions under high-P,T conditions, the inflow-outflow balance strongly suggests that distinct amounts of carbonate minerals may be transported to greater depths.

Since volatile (and life essential) components like carbon dioxide, similar to water, are thought to significantly influence the melting points, density, and viscosities of the Earth's deep interior, their circulation is crucial for understanding the deep Earth dynamics as well as the Earth's habitability. Therefore, the high-P,T phase equilibria of carbon dioxide  $\text{CO}_2$  and major carbonate minerals,  $\text{CaCO}_3$  and  $\text{MgCO}_3$ , have been extensively studied. These prior studies revealed that while the magnesite phase of  $\text{MgCO}_3$  remains stable up to  $\sim 90$  GPa without any phase transition,  $\text{CaCO}_3$  changes its structure continuously in the mantle pressure range, starting from calcite and aragonite to the P21/c-high structure, and more recently, novel high-pressure Ca carbonate phases with exotic compositions not seen at ambient pressure, such as  $\text{CaC}_2\text{O}_5$  and  $\text{CaSiC}_2\text{O}_7$ , have been discovered. This rich evolution of high-pressure Ca carbonate phases suggests that Ca carbonates may become more stable than Mg carbonates under high pressure. However, first-principles calculations evaluating the stability of various hypothetical reactions has reported that  $\text{MgCO}_3$  is only the stable phase at deep mantle temperatures as suggested by experiments. In this study, I re-examined the stability of these diverse high-pressure carbon dioxide and carbonate mineral phases using the first-principles technique. The new results indicate, in contrast to the previous thoughts, the stabilization of Ca-carbonate rather than Mg one at the Earth's core-mantle boundary pressure when they react with subducted crustal components.