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Novel stable compounds in the Mg-Si-O system under exoplanet pressures and their implications in planetary science HAIYANG NIU, State Univ of NY- Stony Brook, ARTEM OGANOV, Skolkovo Institute of Science and Technology, XINGQIU CHEN, DIANZHONG LI, Institute of Metal Research —

The Mg-Si-O system is the major Earth and rocky planet-forming system. Here, through quantum variable-composition evolutionary structure explorations, we have discovered several unexpected stable binary and ternary compounds in the Mg-Si-O system. Besides the well-known SiO_2 phases, we have found two extraordinary silicon oxides, SiO_3 and SiO, which become stable at pressures above 0.51 TPa and 1.89 TPa, respectively. In the Mg-O system, we have found one new compound, MgO_3, which becomes stable at 0.89 TPa. We find that not only the $(MgO)_x(SiO_2)$y compounds, but also two $(MgO_3)_x(SiO_3)_y$ compounds, $MgSi_3O_{12}$ and $MgSiO_6$, have stability fields above 2.41 TPa and 2.95 TPa, respectively. The highly oxidized $MgSi_3O_{12}$ can form in deep mantles of mega-Earths with masses above 20 $M_\oplus$ ($M_\oplus$:Earth's mass). Furthermore, the dissociation pathways of pPv-$MgSiO_3$ are also clarified, and found to be different at low and high temperatures. The low-temperature pathway is $MgSiO_3 \Rightarrow Mg_2SiO_4 + MgSi_2O_5 \Rightarrow SiO_2 + Mg_2SiO_4 \Rightarrow MgO + SiO_2$, while the high-temperature pathway is $MgSiO_3 \Rightarrow Mg_2SiO_4 + MgSi_2O_5 \Rightarrow MgO + MgSi_2O_5 \Rightarrow MgO + SiO_2$. Present results are relevant for models of the internal structure of giant exoplanets, and for understanding the high-pressure behavior of materials.

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