Abstract Submitted
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Stability of dense liquid carbon dioxide[1] BRIAN BOATES, Lawrence Livermore National Laboratory, Dalhousie University, AMANUEL TEWELDE-BERHAN, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory, Dalhousie University — We have used first-principles molecular dynamics to identify a transition from molecular liquid CO2 to a new polymeric liquid phase under compression. The phase transition is first-order and unlike other such transitions, is not accompanied by metallization. The region near the liquid-liquid-solid triple point is particularly interesting as it coincides with pressure-temperature conditions inside the Earth's mantle. We have characterized the stability of CO2 under these conditions; contrary to previous studies, our calculations show that CO2 does not phase separate into carbon and oxygen. Comparisons with and alternative interpretations of previous measurements will be presented. Routes for experimental detection of our predictions will also be discussed.

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