Abstract Submitted
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Ab-initio study on the crystal structure and the superconductivity of calcium in phase IV and V TAKAHIRO ISHIKAWA, HITOSE NAGARA, KOICHI KUSAKABE, Graduate School of Engineering Science, Osaka University, NAOSHI SUZUKI, Department of Pure and Applied Physics, Kansai University — Calcium shows interesting structural phase transitions and the superconductivity under high pressure. Structural transformations from the simple cubic structure (Ca-III) to a complex structure (Ca-IV) at 113GPa and from Ca-IV to another complex one (Ca-V) at 139GPa have been reported, but their structures have not been identified. The pressure-induced superconducting transition has been observed in Ca-III, and the superconducting transition temperature T_c dramatically increases at the transition from Ca-III to Ca-IV and reaches to 25K, which is the highest T_c in an element, at 161GPa in Ca-V. We explored the structures of Ca-IV and Ca-V via the metadynamics simulation based on the density functional theory and obtained two new structures: A helical structure and a zigzag structure. From comparison of the x-ray diffraction patterns we identified that the helical structure and the zigzag structure are candidate structures of Ca-IV and Ca-V, respectively. For the zigzag structure of Ca-V we calculated T_c using the Allen-Dynes formula. We assumed the effective screened Coulomb repulsion constant μ^* to be 0.1. We obtained T_c=18.19K at 140GPa, and the estimated values of T_c are high and are close to the experimental values of Ca-V.

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