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Ab initio calculations of structural phase transitions of XP compounds (X=La, Ce, Pr, and Nd) under high pressure

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Lanthanide-monophosphate materials have been used in many applications, such as scintillators for detecting radiation and inorganic fluorescent labels. In this work, high-pressure phase transitions of XP (X = La, Ce, Pr, and Nd) have been undertaken. Based on density functional theory (DFT), the energetic stability of XP materials were investigated to verify the most stable structures at pressure ranges. NaCl-type, CsCl-type, PbO-type, and P4/mmm which are based on related experimental results, were chosen to carry out in all XP materials. Using local density approximation (LDA), the results reveal that all compounds exhibit the NaCl-type structure at ambient pressure which is in good agreement with the experiments. LaP, CeP and NdP transform by the path of NaCl-type → PbO-type → CsCl-type structure. Moreover, CeP continuously undergoes the transformation to P4/mmm structure. In contrast, PrP passes P4/mmm phase before approaching PbO-type structure. Electronic density of states (DOS) and band structures were performed to clarify the phenomenon of high-pressure phase transitions of these compounds.

Primary author: Mr SAINAMTHIP, Chirayu (Mahidol Wittayanusorn School, Nakhon Pathom 73170, Thailand)

Co-authors: Mr KOTMOOL, Komsilp (Department of Physics, Mahidol Wittayanusorn School, Nakhon Pathom 73170 Thailand; Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand); Mr JIMLIM, Pornmongkol (Department of Physics, Mahidol Wittayanusorn School, Nakhon Pathom 73170, Thailand); BOVORNRATANARAKS, Thiti (Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand)

Presenter: Mr SAINAMTHIP, Chirayu (Mahidol Wittayanusorn School, Nakhon Pathom 73170, Thailand)

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