

Abstract Submitted
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Origins of charge density wave in novel Pt-based superconductors: SrPt₂As₂ and LaPt₂Si₂ SOORAN KIM, KYOO KIM, B.I. MIN, POSTECH — The intriguing coexistence of the charge density wave (CDW) and superconductivity in SrPt₂As₂ and LaPt₂Si₂ has been investigated by using the ab initio density functional theory band structure and phonon calculations. We have found that the local split distortions in the [As-Pt-As] layers play an essential role in driving the five-fold supercell CDW instability as well as the phonon softening instability in SrPt₂As₂. In contrast to SrPt₂As₂, the CDW and phonon softening instabilities in LaPt₂Si₂ occur without split positions of Pt, indicating that the driving mechanisms of the CDW in SrPt₂As₂ and LaPt₂Si₂ are different. The phonon calculations, however, suggest that the CDW and the superconductivity coexist in [X-Pt-X] layers (X = As or Si) in both cases.

Sooran Kim
POSTECH

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