Origins of charge density wave in novel Pt-based superconductors: SrPt\(_2\)As\(_2\) and LaPt\(_2\)Si\(_2\) 

SOORAN KIM, KYOO KIM, B.I. MIN, POSTECH — The intriguing coexistence of the charge density wave (CDW) and superconductivity in SrPt\(_2\)As\(_2\) and LaPt\(_2\)Si\(_2\) 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 SrPt\(_2\)As\(_2\). In contrast to SrPt\(_2\)As\(_2\), the CDW and phonon softening instabilities in LaPt\(_2\)Si\(_2\) occur without split positions of Pt, indicating that the driving mechanisms of the CDW in SrPt\(_2\)As\(_2\) and LaPt\(_2\)Si\(_2\) 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.