

# Highlights

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## Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure

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Pressure-induced superconductivity and structural phase transitions in phosphorus (P) are studied by resistivity measurements under pressures up to 170 GPa and by fully *ab initio* crystal structure exploration and superconductivity calculations up to 350 GPa.

Two distinct superconducting transition temperature (TC) vs pressure (P) trends at low pressure have been reported more than 30 years ago, and we are able to devise a consistent explanation founded on thermodynamically metastable phases of black phosphorus. Our experimental and theoretical results form a single, consistent picture which not only provides a clear understanding of elemental P under pressure but also sheds light on the longstanding and unsolved *anomalous* superconductivity trends. Moreover, at higher pressures we predict a similar scenario of multiple metastable structures which coexist beyond their thermodynamical stability range. We observe that all the metastable structures systematically exhibit larger transition temperatures than the ground-state structures, indicating that the exploration of metastable phases represents a promising route to design materials with improved superconducting properties.

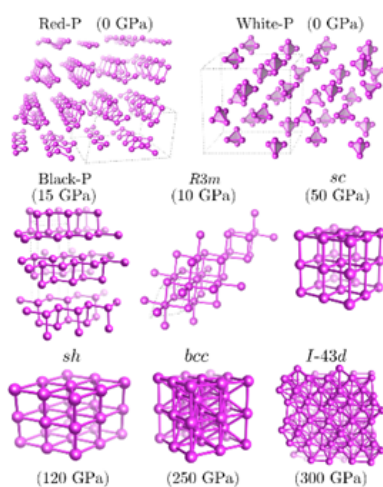


Fig.1: Crystal structure of phosphorus at indicated pressures

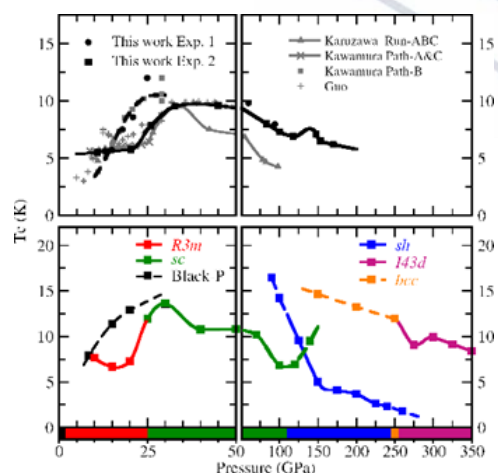


Fig.2: Experimental (top panels) and theoretical superconducting (bottom panels) critical temperatures.