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High pressure superconducting phase of Sulfur and Phosphorus

GIANNI PROFETA, Department of Physical and Chemical Sciences, University of L'Aquila — The recent discovery of very high superconducting critical temperature in high pressure phases of SH_3 and PH_3 opens new perspectives on the research of superconducting materials under high pressure and poses important and stringent conditions on the theoretical predictions of crystal structures and superconducting critical temperatures (T_c). In the same high pressure runs for SH_3 and PH_3 , the superconducting phase diagram of both elemental sulfur and phosphorus have been re-examined, revealing peculiar features which calls for a complete theoretical explanation. In sulfur a discontinuity of T_c as a function of the pressure (P) is observed, while the $T_c(P)$ curve in phosphorus strongly depends on the initial experimental conditions. In this talk, by means of first principles superconducting DFT, we predict the superconducting phase diagram of elemental sulfur and phosphorus under high pressure with unprecedented agreement with available experimental results. We discovered that the discontinuity of $T_c(P)$ in sulfur arises from peculiar and unexpected multiband effects, while the presence of metastable phases explain the puzzling $T_c(P)$ curves in phosphorus.

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