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Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen

P. Cudazzo[1], G. Profeta[1], A. Sanna[2,3], A. Floris[3], A. Continenza[1], S. Massidda[2], and E. K. U. Gross[3]

[1]*CNISM - Dipartimento di Fisica, Università degli Studi dell'Aquila, Via Vetoio 10, I-67010 Coppito (L'Aquila) Italy*

[2]*SLACS-INFM/CNR—Dipartimento di Fisica, Università degli Studi di Cagliari, I-09124 Monserrato (CA), Italy*

[3]*Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany*

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We present a first-principles study of the electron-phonon interaction and the prediction of the superconducting critical temperature in molecular metallic hydrogen. Our study is able to single out the features which drive the system towards superconductivity: mainly, a rich and complex Fermi surface and strongly coupled phonon modes driving the intra- or intermolecular charge transfer. We demonstrate that in this simple system, a very high superconducting critical temperature can be reached via electron-phonon and Coulomb electron-electron interactions.

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