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Low-temperature metallic liquid hydrogen: an ab-initio path-integral molecular dynamics perspective JI CHEN, XIN-ZHENG LI, QIAN-FAN ZHANG, ICQM and School of Physics, Peking University, MATTHEW PROBERT, Department of Physics, University of York, CHRIS PICKARD, Department of Physics and Astronomy, University College London, RICHARD NEEDS, Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, ANGELOS MICHAELIDES, London Centre for Nanotechnology and Department of Chemistry, University College London, ENGE WANG, ICQM and School of Physics, Peking University — Experiments and computer simulations have shown that the melting temperature of solid hydrogen drops with pressure above about 65 GPa, suggesting that a low temperature liquid state might exist. It has also been suggested that this liquid state might be non-molecular and metallic, although evidence for such behaviour is lacking. Using a combination of ab initio path-integral molecular dynamics and the two-phase methods, we have simulated the melting of solid hydrogen under finite temperatures. We found an atomic solid phase from 500 to 800 GPa which melts at < 200 K. Beyond this and up to pressures of 1,200 GPa a metallic atomic liquid is stable at temperatures as low as 50 K. The quantum motion of the protons is critical to the low melting temperature in this system as ab initio simulations with classical nuclei lead to a considerably higher melting temperature of $\sim$300 K across the entire pressure range considered.

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