Metastable states on the pressure isotherms of warm dense cesium

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Ab initio molecular dynamics of warm dense cesium gives two values of the pressure on one isotherm and thus reveals metastable states in the region of a possible plasma phase transition [1]. Those calculations yield only the metastable states on the branch of higher pressure. An on-the-fly machine-learning potential extends the calculation to a wide region of the phase diagram and to a larger number of particles. The metastable states on the branch of lower pressure are obtained in this work by expanding the simulation cell along an isotherm. Since the electronic temperature is equal to ionic temperature, a separate potential is fitted to each isotherm. As the temperature rises, the region of metastability shifts toward higher densities, in contrast to warm dense hydrogen.

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