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Multi-center semi-empirical quantum models for carbon under extreme thermodynamic conditions[1] NIR GOLDMAN, Lawrence Livermore Natl Lab — We report on the development of many-body density functional tight binding (DFTB) models for carbon accurate over thousands of GPa and tens of thousands of Kelvin. DFTB holds promise as a fast quantum simulation approach that can yield several orders of magnitude increase in computational efficiency over Kohn-Sham Density Functional Theory (DFT) while retaining most of its accuracy. However, standard DFTB can yield large errors for materials under high pressures and temperatures, where electrons can become delocalized. Here, we overcome these limitations by computing the environmental dependence of the DFTB Hamiltonian matrix elements directly from DFT. We include these results in DFTB calculations by either explicitly calculating three-center terms in the Hamiltonian, or by implicitly incorporating them in the diagonal matrix elements. We then determine a three-body repulsive energy for the implicit approach, which yields accurate equation of state and structural properties for both solid and metallic liquid states of carbon. Our new models exhibit a straightforward method by which many-body effects can be included in DFTB, thus extending it to the time scales of current compression experiments, where physical and chemical properties can be difficult to interrogate directly.

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