

Transferability of Carbon Interatomic Potentials: Lessons from Amorphous Carbon & Graphitization

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Assessing the transferability of a potential is a challenging and sometimes thankless task. Over the last couple of years we have used LAMMPS to perform an ongoing systematic comparison of 14 common potentials for carbon, ranging from the original Tersoff and REBO methods to modern approaches employing screening and machine learning. Amorphous carbons generated by liquid quenching and graphitization induced by annealing provide a vigorous test of bond-making and bond-breaking processes, and reveal disturbingly large differences between potentials. In many cases the variability can be traced to the level of sophistication of the potential, providing an impetus for future developments. While not perfect, the Environment Dependent Interaction Potential (EDIP) developed by the author provides surprisingly good performance in many contexts. Some recent applications of EDIP are presented, in particular radiation damage in graphite and structure generation of nanoporous carbons.