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Choosing a Classical Potential in Multi-Scale Modeling ADITI MALLIK, Physics, University of Florida, KRISHNA MURALIDHARAN, DECARLOS TALYOR, KEITH RUNGE, JAMES DUFTY — For problems relating to fracture in multi-scale modeling, a consistent embedding of a quantum (QM) domain in its classical (CM) environment requires that the classical potential chosen for the CM region should yield the same geometry and elastic properties as the QM domain. It is proposed that such a classical potential can be constructed using *ab initio* data on the equilibrium structure and weakly strained configurations calculated from the quantum description, rather than the more usual approach of fitting to a wide range of empirical data. This scheme is illustrated in detail for a model system, a silica nanorod that has the same stiochiometric ratio of Si:O as observed in real silica. The potential is chosen to have the same functional form as TTAM but the parameters are fitted using a genetic algorithm with force data obtained from a quantum calculation. The Young's modulus (Y) obtained from this classical potential matches closely with that obtained from the QM method for strains up to 10%, unlike the standard TTAM which differs by 18%. Furthermore, the bond lengths and bond angles in the rod are an order of magnitude more accurate for the new potential in comparison to that from the current TTAM or BKS potential parameters. This potential provides a "seamless" coupling between the QM and CM regions in applications of QM/CM multi-scale modeling for this silica nanorod. The wider application of this potential can be found in glasses.

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