Concepts of Multi-Scale Modeling A. MALLIK, University of Arizona, K. RUNGE, J.W. DUFTY, University of Florida — The approximate representation of a quantum solid as an equivalent composite semi-classical solid is considered. In the classical bulk domain this potential energy is represented by potentials constructed to give the same structure and elastic properties as the underlying quantum solid. In a small local quantum domain the potential is determined from a detailed quantum calculation of the electronic structure.The features of this problem are the representation of the classical domain by potentials focused on reproducing the specific quantum response being studied, development of 'pseudo-atoms' for a realistic treatment of charge, and inclusion of polarization effects on the quantum domain due to its distant bulk environment

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