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Multi-Scale Modeling from First-Principles

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Electronic structure theory (the nature of the chemical bond) is the base and the finest scale for multi-scale modeling of the function of materials. Frequently it is assumed that details at this base do not matter when length and time scales approach meso- or macroscopic proportions (e.g. μm and minutes). In this talk I will show for various examples that details matter indeed. When accuracy is lacking at the base, there is little hope for predictive results at any level of modeling that follows. I will also emphasize the importance of reversible mapping and error control between the different levels of multi-scale modeling when moving up the chain of methods to successively increasing spatial and temporal dimensions. – In this context I will also address the sometimes problematic accuracy of present day density functional theory methods and show how it can be determined and errors corrected.