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Ultracold Molecules in Crystals of Light: A Highly Tunable System for Exploring Novel Materials, Quantum Dynamics, and Quantum Complexity[1] LINCOLN CARR, KENJI MAEDA, Colorado Sch of Mines, MICHAEL L. WALL, JILA, NIST and U. Colorado Boulder — Ultracold molecules trapped in optical lattices present a new regime of physical chemistry and a new state of matter: *complex dipolar matter*. Such systems open up the prospect of tunable quantum complexity. We present models for the quantum many-body statics and dynamics of present experiments on polar bi-alkali dimer molecules. We are developing Hamiltonians and simulations for upcoming experiments on dimers beyond the alkali metals, including biologically and chemically important naturally occurring free radicals like the hydroxyl free radical (OH), as well as symmetric top polyatomic molecules like methyl fluoride (CH_3F). These systems offer surprising opportunities in modeling and design of new materials. For example, symmetric top polyatomics can be used to study quantum molecular magnets and quantum liquid crystals. We use matrix-product-state (MPS) algorithms, supplemented by exact diagonalization, variational, perturbative, and other approaches. MPS algorithms not only produce experimentally measurable quantum phase diagrams but also explore the dynamical interplay between internal and external degrees of freedom inherent in complex dipolar matter. We maintain open source code (openTEBD and openMPS) available freely and used widely.

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