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Abstract for an Invited Paper
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Accelerated Molecular Dynamics of Rare Events with the Bond-Boost Method[1]

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A continuing challenge in materials simulation is to conduct long time and large length simulations of structural evolution, while accurately retaining atomic detail. For many materials, dynamical evolution occurs through a series of "rare events," in which the system spends a long-time period in one free-energy minimum before escaping and moving on to another. To address the rare-event problem for materials evolution, we developed the bond-boost method, which is a variant of hyperdynamics. We will introduce the bond-boost method and demonstrate several applications of it to thin-film growth and surface kinetics. A significant problem that plagues rare-event simulations is the "small barrier problem" and we will discuss how this problem can be addressed within the bond-boost method. We will also discuss our recent efforts to combine this method with kinetic Monte Carlo simulations.

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