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Using Molecular Simulation to Develop New Materials for Energy and Environmental Applications[1]

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We face two enormous challenges in the coming decades. First, we must find ways to provide clean, affordable energy to an ever-growing population. Second, as underdeveloped countries advance, we must find ways to provide access to advanced technologies that enhance human wellbeing. What makes these two challenges even more daunting is that they both must be met using sustainable technologies; simply relying on old dirty technologies is not an option. In this talk, I will show how approaches rooted in chemical physics are being used to develop new materials that can be used to meet these challenges. In particular, I will give examples where molecular-based simulations are being used in three areas: 1) the discovery of new ionic liquid solvents for capturing CO2 produced from fossil fuel combustion; 2) the development of new refrigerants that have better performance and significantly lower global warming potentials than existing refrigerants; and 3) fundamental investigations of actinide ions in solution, with the objective of developing new separation processes for nuclear waste remediation and fuel reprocessing technologies.

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