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**First Principles based methods and applications for realistic simulations on complex soft materials
to develop new materials for energy, health, and environmental sustainability**

WILLIAM GODDARD, California Institute of Technology

For soft materials applications it is essential to obtain accurate descriptions of the weak (London dispersion, electrostatic) interactions between nonbond units, to include interactions with and stabilization by solvent, and to obtain accurate free energies and entropic changes during chemical, physical, and thermal processing. We will describe some of the advances being made in first principles based methods for treating soft materials with applications selected from new organic electrodes and electrolytes for batteries and fuel cells, forward osmosis for water cleanup, extended matter stable at ambient conditions, and drugs for modulating activation of GCPR membrane proteins,