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Advancing the Design of Batteries through Atomic-Scale Modeling of Materials

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Atomic-scale modeling empowers researchers and engineers to rapidly and cost-effectively explore mechanisms and properties of existing materials and to propose new materials for every battery component. We will illustrate the capabilities of atomistic simulations with case studies from our industry research portfolio. In this presentation we show how calculations of heats of formation, redox potentials, and reaction energies can be used to predict the electrochemical stability of materials and give insight into which new phases and compounds are formed in redox reactions at the electrodes. Existing and formed phases are characterized with calculated IR/Raman spectra, NMR data, and UV-Vis absorption. With accurate calculations of elastic properties [1] related to brittleness, ductility, and hardness in addition to thermal expansion and volume changes, we can identify mechanical mismatches and stress which can cause loss of interfacial contact and, hence, delamination. All calculations are performed with the software environment MedeA® [2,3] which integrates the best simulation approaches with comprehensive databases, efficient computing and analysis tools, and utilities to convert results from simulations into innovative materials formulations.

REFERENCES

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