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The shape of things to come: some thoughts and plans for computational condensed matter physics

Computational science has become one of the greatest accelerators of research, with results and impact that run deep in science and technology. For condensed matter physics, the key challenges are those of predictive accuracy, with simulations able to capture the quantum and correlated nature of electrons and nuclei; of realistic complexity, aiming to describe ever more closely the macroscopic world; and of materials informatics, leveraging the disruptive capabilities of machine learning and artificial intelligence.

I'll highlight some of the key efforts we are targeting: addressing the electronic structure of compounds with strongly localized and correlated electrons, developing mesoscopic equations and formulations that bring atomistic and quantum precision to the macroscopic scale, and delivering automated capabilities that can be externalized and then orchestrated by human and not-so-human players.

Some example applications will cover materials for energy (Li-ion cathodes and solid-state conductors) and materials for information-and-communication technologies (2D and 1D materials, topological insulators, and superconductors).