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PLENARY: Efficient and accurate first-principles predictions of structures and energies for Materials Science, Chemistry and Biology

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Abstract content
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In materials science, chemistry, and biology, it is of critical importance to know if one atom or molecule can bind to another and with how much energy. The strengths of different types of bonds between atoms and molecules can vary from several meV to several eV. Although some first-principles methods can provide accurate descriptions of all bond types, those methods are not efficient enough for studies of complex systems (e.g., large systems, ab initio molecular dynamics, and high-throughput searches for functional materials). We show here that the recently developed non-empirical strongly constrained and appropriately normed (SCAN) meta-generalized gradient approximation (meta-GGA) within the density functional theory framework predicts accurate geometries and energies of diversely-bonded molecules and materials (including covalent, metallic, ionic, hydrogen, and van der Waals bonds), significantly improving over its predecessors, at comparable efficiency, the GGAs that dominate materials computation. Often SCAN matches or improves upon the accuracy of a computationally expensive hybrid functional, at almost-GGA cost. SCAN captures the intermediate-range van der Waals (vdW) interaction, which is largely missed by the conventional GGAs and hybrid functionals. The addition of the long-range vdW correction to SCAN results in a versatile vdW functional that is accurate and outperforms its competitors for a variety of vdW-dominated systems, including layered materials and organic molecules adsorbed on metal surfaces.

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