Automated Quantum Chemistry for Chemical Discovery

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The potential energy surface (PES) of a molecule (or supermolecule) contains all the information needed to understand its ground-state chemistry completely. Despite this fact, few chemical reactions are discovered using theory. Even when a reaction is already known, producing a mechanism, potential-energy diagram, thermochemistry, and simple rate constants is laborious. This labor can be automated. A major result of such automation will be to empower non-experts to use quantum methods for discovering new chemistry and for understanding known reactions.