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Basc: Applying Bayesian optimization to the search for global minima on potential energy surfaces
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AFFILIATIONS: Washington University, 1 Brookings Dr., St. Louis, MO, United States
ABSTRACT: We present a novel application of Bayesian optimization to the field of surface science: rapidly and accurately searching for the global minimum on potential energy surfaces. Controlling molecule-surface interactions is key for applications ranging from environmental catalysis to gas sensing. We present pragmatic techniques, including exploration/exploitation scheduling and a custom covariance kernel that encodes the properties of our objective function. Our method, the Bayesian Active Site Calculator (BASC), outperforms differential evolution and constrained minima hopping - two state-of-the-art approaches - in trial examples of carbon monoxide adsorption on a hematite substrate, both with and without a defect.
INDEX KEYWORDS: Artificial intelligence; Carbon; Carbon monoxide; Evolutionary algorithms; Global optimization; Learning systems; Molecular physics; Optimization; Potential energy surfaces; Quantum chemistry, Bayesian optimization; Carbon monoxide adsorption; Covariance kernel; Differential Evolution; Environmental catalysis; Exploration/exploitation; Novel applications; Objective functions, Potential energy
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