Modified ARTn method for efficient surface transition state identification

This paper addresses the challenge of exploring potential energy surfaces to understand chemical reactions on surfaces, which is crucial for applications in catalysis, corrosion, and thin-film growth. Traditional methods such as the Activation-Relaxation Technique (ARTn) often struggle to identify transition states in complex surface reactions due to high computational demands and difficulties in navigating intricate energy landscapes. To overcome this, the study introduces iso-ARTn method, which utilizes constraints on an orthogonal hyperplane and an adaptive active volume to enhance search efficiency. When applied to a Pt(111) surface with 0.3 monolayers of oxygen coverage using a neural network potential, iso-ARTn achieved an 8.2% higher success rate and required 40% fewer force evaluations than the original ARTn. Moreover, combined with kinetic Monte Carlo simulation for Pt(111) oxidation, iso-ARTn revealed the structure consistent with experimental observations. This study paves the way for investigating complex surface processes by efficiently identifying elementary reactions through improved saddle point search. This work was published in Journal of Chemical Theory and Computation 2024, **20**, 8024.