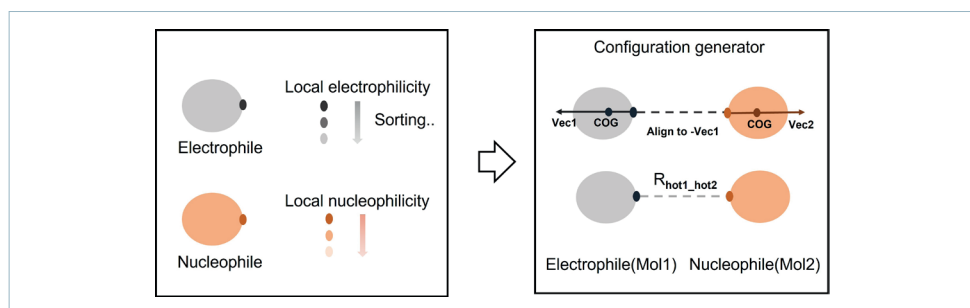
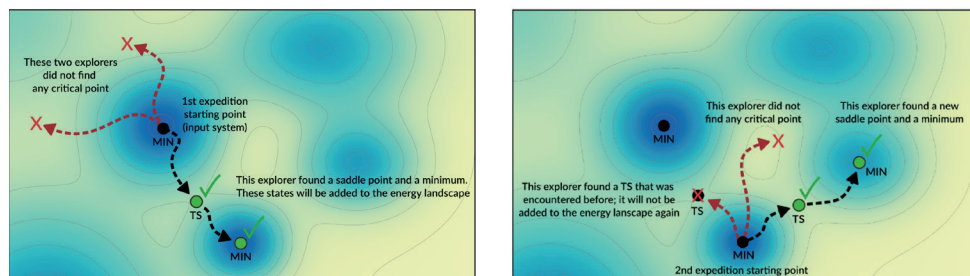


DISCOVERY OF DEGRADATION MECHANISMS OF ELECTROACTIVE MOLECULES

Electrolyte degradation is a major challenge for organic redox flow batteries. The ability to predict the corresponding reaction mechanisms of great value to mitigate the degradation. Our algorithm is a valuable tool for the automated discovery of degradation pathways.



Automatically generate encounter complexes based on electro-/nucleophilicity descriptors

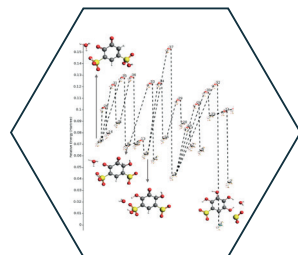
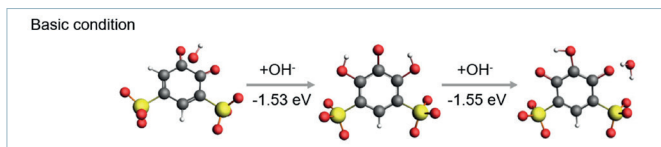
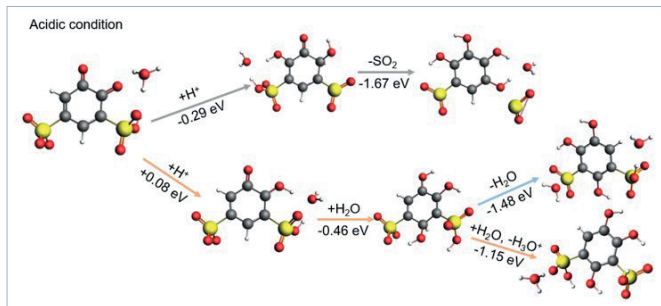


Automatically explore the potential energy surface of a given system by searching for nearby critical points (local minimum or saddle points)



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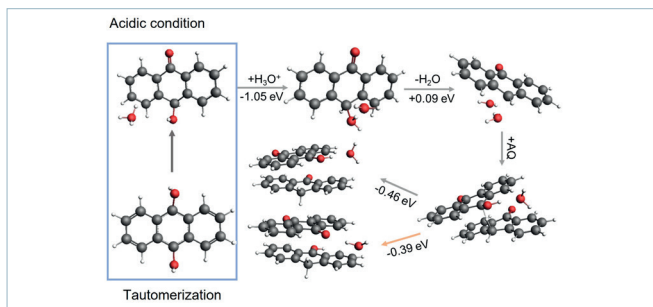
Acid-/base-catalyzed degradation of BQDS



MORE:
Acid-/Base
catalyzed DHDMBS

Using our algorithm, we successfully mapped out a full reaction network of

- substituted quinones under acidic/basic conditions
- disproportionation reaction of anthrahydroquinone under acidic condition.



Disproportionation
Reaction

Discovering new
degradation
mechanisms...

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