Abstract for AVS71

Activation of C-X bonds on transition metal surfaces: Insight from DFT studies

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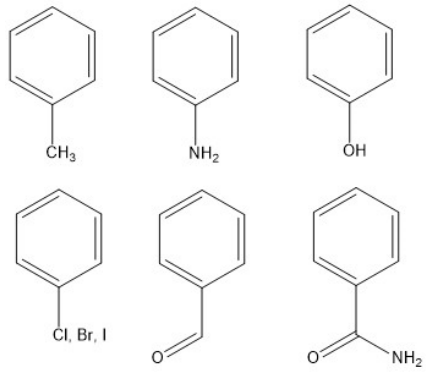


Figure 1. Set of functionalized benzene-based small molecule inhibitors (SMIs) considered in this study.

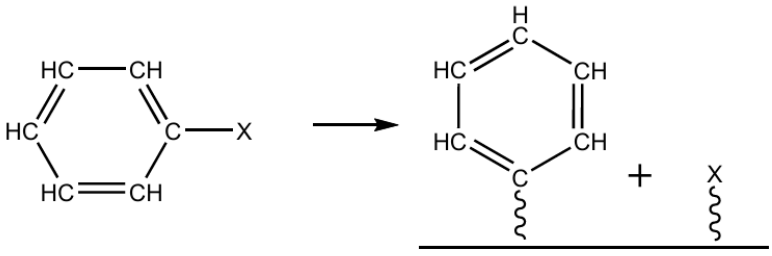
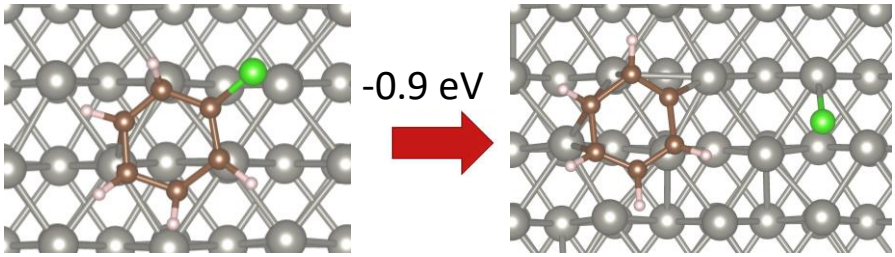


Figure 2. General reaction scheme for surface-mediated dissociation of SMIs via C–X bond cleavage.



on W	HOMO-LUMO Gap (eV)	Adsorption Energy (eV)	Reaction Energy (eV)
Cl-Benzene	4.6	-3.3	-0.9
Br-Benzene	4.5	-3.4	-1.0
I-Benzene	4.1	-3.6	-1.1

Figure 3. Snapshots from 800K AIMD simulation showing the energy profile of Cl-transfer to the W surface. Summary of electronic and thermodynamic properties for halo-benzenes de halogenation.

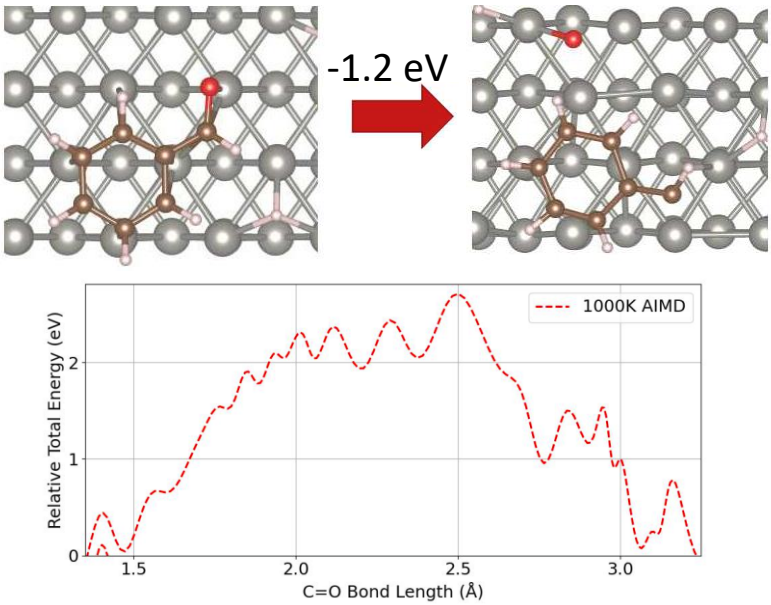


Figure 4. Snapshots from 1000K AIMD simulation showing the energy profile of O-transfer to the W surface. The optimized dissociated adsorbed state is 1.2 eV more stable than the initial state.