A first-principles study of the catalytic hydrodechlorination of 1,2-dichloroethane

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Chlorinated hydrocarbons are common intermediates and by-products from various chemical processes. Industrial chlorocarbon wastes are serious environmental pollutants, and an efficient treatment method is highly desired [1]. The catalytic hydrodechlorination, which utilizes hydrogen to convert chlorinated species into hydrogen chloride and valuable hydrocarbon products, is an attractive approach from both the economic and environmental standpoints. Catalytic hydrodechlorination of 1,2-dichlorethane produces both ethylene and ethane, and thus poses an additional challenge of selectivity, where ethylene, due to its higher economic value, is the desired product over ethane.

Here we aim to investigate the hydrodechlorination of 1,2-dichloroethane over transition metal surfaces. Past studies have shown that bimetallic catalysts yield good catalytic performance in terms of both the dechlorination activity and the ethylene selectivity [2]. The lack of fundamental understanding of the reaction mechanism and the catalytic behavior, however, hinders catalyst design and optimization. Therefore, we adopted a first-principles approach in our study. Through density functional theory calculations, we evaluate the energetics of adsorbates and reactions over metal surfaces. The results offer valuable insights into the surface reaction mechanism and will potentially facilitate the rational design of optimal catalysts. This presentation will demonstrate the trend of hydrodechlorination reactivity over a series of monometallic surfaces, followed by a detailed mechanistic study on platinum catalysts.

[1] E. D. Goldberg, Halogenated hydrocarbons: past, present and near-future problems, *Science of the Total Environment* **100**, 17-28 (1991).
[2] V. I. Kovalchuk and J. L. d'Itri, Catalytic chemistry of chloro- and chlorofluorocarbon dehalogenation: from macroscopic observations to molecular level understanding, *Applied Catalysis A: General* **271**, 13-25 (2004).