# Catalytic De-halogenation of Halogen-containing Solid Wastes by Transition Metal Oxides

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Catalytic co-pyrolysis of halogenated compounds with electric arc furnace dust (EAFD) constitutes an effective disposal strategy regarding energy recovery and environmental safeguard. However, despite many detailed experimental investigations over the last few years; the specific underlying mechanism of the reactions between the halogen laden materials with EAFD remain largely poorly understood. In this contribution, systematic theoretical thermo-kinetic investigations were performed using the accurate density functional theory calculations to understand, on a precise atomic scale, the reaction mechanisms of major products from thermal decomposition of polyvinyl chloride (PVC) and brominated flame retardants (BFRs) with nanostructures (clusters and surfaces) of hematite ($\alpha$-$Fe_2O_3$), zincite (ZnO) and magnetite ($Fe_3O_4$).

The detailed kinetic analysis indicates that the dissociative adsorption of hydrogen halides molecules, the major halogen fragments from thermal degradation of halogen laden materials, over those metal oxide structures affords oxyhalides structures via modest activation barriers. Transformation of oxyhalides into metal halides occurs through two subsequent steps, further dissociative adsorption of hydrogen halides over the same structures followed by the release of $H_2O$ molecule. In the course of the interaction of halogenated alkanes and alkenes with the selected metal oxide structures, the opening channel in the dissociative addition route requires lower activation barriers in reference to the direct HCl/Br elimination pathways. However, sizable activation barriers are encountered in the subsequent $\beta$ C-H bond elimination step. The obtained accessible reaction barriers for reactions of halogenated alkanes and alkenes with the title metal oxides demonstrate that the latter serve as active catalysts in producing clean olefins streams from halogenated alkanes.