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Chemistry of Al in Oxidizer Medium: From Shock Initiation to Post Detonation Kinetics SANTANU CHAUDHURI, MARTIN LOSADA, SHAHRYAR FOTOVATI, ISP/Applied Sciences Laboratory, Washington State University — Reactive materials, propellants, and thermites are often constructed from Al/oxidizer composites. Al/oxidizer composites are also considered for self-sustaining reactions for deep space applications to reduce the need for carrying oxygen. In particular, Al/Teflon, Al/I_2O_5 and Al/RDX composites will be discussed as representative Al in oxidizer systems. Results of post-detonation kinetics using transition state theory and master equation based RRKM theory will be compared including discussion on some unresolved theoretical issues in collision theories and basis set effects in predicting the temperature/pressure-dependent kinetics. For Al/Teflon system, the RRKM theory calculated fall-off curves show a significant pressure dependence of rate constant in wide range of 0-1 MPa pressures at elevated temperatures. For Al/I_2O_5 systems, incorporation of spin-orbit coupling in DFT with various standard and augmented basis sets is important. A mechanism for generation of I_2 and O_2 during the reaction will be proposed. Finally, describing shock initiation reactions inside a condensed phase Al/RDX composites for a combustion reaction or detonation is currently a challenge for theoretical chemistry and chemical dynamics community. Especially, exact theoretical treatment for kinetics of reactants in confined hot-spots under high-pressure/temperature conditions is lacking. A new collision theoretical approach and reactive embedding possiblityies will be discussed as alternative to reactive force field based simulations of hot-spot growth.

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