HYPERVELOCITY IMPACT EFFECTS ON SPACE MISSION INSTRUMENTATION. A. Jaramillo-Botero[1] [ajaramil@caltech.edu], L.W. Beegle[2] [luther.w.beegle@jpl.nasa.gov], R.P. Hodyss[2] [robert.p.hodyss@jpl.nasa.gov], W.A. Goddard III[1] [wag@wag.caltech.edu], and M.R. Darrach[2] [murray.r.darrach@jpl.nasa.gov], [1]California Institute of Technology, 1200 E California Blvd, Pasadena, CA 91125, [2]Jet Propulsion Laboratory, 4800 Oak Grove Dr, Pasadena, CA 91109

Introduction: Understanding the physics and chemistry of hypervelocity collisions of small impactors on spacescrafts and their instruments is critical to their survival and operational accuracy. Unfortunately, high impact energies from small particles (e.g. organic species or cosmic dust) lead to untraceable adiabatic and non-adiabatic chemical events that render conventional experimental and modeling techniques impractical, such as ionizing fragmentation. Recent modeling and simulation breakthroughs at Caltech, namely, the first-principles-based electron force field (eFF)[1,2] and the ReaxFF[3] reactive force field have provided an unprecedented opportunity for accurately describing the energetics and fragmentation phenomena during hypervelocity impact on space vehicles and their on-board instruments. Here we used ReaxFF and eFF to study the complex fragmentation pathways of molecular species impacting Cassini's ion and neutral mass spectrometer during its flybys through Enceladus and Titan, two of Saturn's moons, and to provide material/geometry related predictions for Europa's mission mass analyzer.

Reactive dynamics modeling methods: ReaxFF provides nearly the accuracy of ground state quantum mechanics (QM) for describing large-scale reactive processes at computational costs comparable to conventional non-reactive force fields. It is the combination of simulating reactivity, diffusion, material decohesion, and phase transitions that enables an accurate description of complicated chemical events associated with varying temperature gas-phase reactions, surface chemistry, transport and flow of reactive species across the material surfaces and interfaces. The functional forms in ReaxFF give accurate descriptions of transition states for allowed and forbidden reactions, consisting of bond order dependent valence terms, environmentally dependent charge distributions, and non-bond or van der Waals (vdw) interactions between all atoms. For extreme conditions, i.e. in which non-adiabatic phenomena related to electronic excitations dominate (e.g. ionization fragmentation), ReaxFF becomes inaccurate. At such energies, eFF provides a cost-effective quantum-based solution to studying the dynamics of large-scale electronic excitations, providing a powerfull tool for predicting non-adiabatic phenomena under true space mission conditions. With eFF, electrons are explicitly included in the dynamical equations, but instead of solving the time-dependent Schrödinger equation, we write the many-electron wavefunction as a Hartree product of floating Gaussian wavepackets, one for each electron, and propagate the dynamics as the electrons and nuclei interact. We use a spin dependent potential to replace the orthogonality induced by the Pauli principle, allowing nonadiabatic transitions to be described. Effective core pseudopotentials (ECP) based on angular momentum projection operators define the high Z Pauli potential for eFF. eFF-ECP leads to accurate geometries and energies for bulk systems and systems containing complex bonding.

Cassini data analysis: The NASA/ESA Cassini probe of Saturn analyzed the molecular composition of plumes emanating from one of its moons, Enceladus, and the upper atmosphere of another, Titan[4]. However, interpretation of this data is complicated by the hypervelocity (HV) flybys of up to ~18 km/sec that cause substantial molecular fragmentation. We have (i) related energy of HV impact to fragmentation for different species relevant to INMS data, (ii) obtained molecular species mixing ratios and mass spectra that compare directly to existing INMS data, (iii) described molecular topology factors that affect fragmentation processes and INMS data interpretation, (iv) identified important species that may be a product of HV impact (e.g., formaldehyde from hydrocarbons), (v) confirmed that NH_3 and other organic species may have been chemisorbed on the TiO_2 INMS detector surfaces during Titan's fly-by, therefore potentially affecting nitrogen-based readouts from Enceladus, and (vi) explored the effect of molecular impact on the chemical and morphological properties of the INMS TiO_2 antechamber walls [5].

Mass Analyzer for Europa Mission: With a spacecraft speed of ~5 to 7 km s^{-1}, atoms and molecules of Europa's sputtered atmosphere will cause surface chemistry or condensed phase chemistry unless these species are directly ionized and detected before they collide with other species/surfaces producing secondary species. Determination of species abundances, both in the ram and wake directions of Europa's orbit around Jupiter, will provide critical information about the dynamic magnetospheric interaction with the icy moon. We have benchmarked the physisorption, chemisorption and fragmentation of H_2O, CO_2, and SO_2, over a range of impact angles and velocities, on two candidate surfaces to determine material and geometric design choices for the instrument's aperture design.

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