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Atomic, Molecular and Plasma-Material Interaction Data for Fusion Science and Technology

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fusion experiments (transport, radiation losses, spectroscopic diagnostics). He concluded that the ways to improve the efficiency of A+M+PMI data use in fusion plasma diagnostics are: (i) creating the simulators (fast-routine simplified computational models), (ii) atomic kinetic models for real-time diagnostics.

J. Tennyson: Electron-molecule collision data using the R-matrix method

Detailed models of molecule-rich regions of fusion plasmas, such as in the divertor, require significant amounts of data on molecular processes. It is extremely difficult to obtain required data from experiment because most species of interest are unstable (radicals) or are otherwise difficult to handle (BeH and BeH_2). Prof Tennyson presented examples of recent electron-molecule calculations for important plasma processes such as vibrational excitation and electron impact dissociation. Quantum mechanical calculations, such as those using R-matrix method in principle provides a way of generating the necessary information. However, theoretical calculations often show strong model dependence, both target model and scattering model and, particularly in situations where they cannot be validated by experiment, it is hard to be specific about the underlying uncertainty in any predicted cross section or rate. He addressed some of the issues raised by these calculations and discussed the prospects for future, fusion-related studies.

A. Laricchiuta: Thermodynamics and transport properties of high-density hydrogen plasma

The development of new technologies and experimental techniques has triggered intensive theoretical research on the modeling of spatially confined quantum systems and also of extreme-high-pressure plasmas like in stellar envelopes. Dr Laricchiuta presented the thermodynamic properties and transport coefficients of non-ideal, high-density hydrogen plasma accounting for quantum effects due to the change in the energy spectrum of atomic hydrogen when the electron-proton interaction is considered embedded in the surrounding particles. The ionization equilibrium is affected by the pressure ionization due to the lowering of the ionization potential. Furthermore the ensemble of levels affects also the internal partition function of H atom in the Saha equation. She reported on the effects of non-ideality in the thermodynamics of high-density hydrogen plasma on transport properties in the frame of the Chapman-Enskog theory. The electrical conductivity of Debye plasma also exhibits a dependence on the total electron density that is affected by the pressure ionization, i.e. the minimum behavior of the conductivity and the *Mott transition* merging to the fully ionized regime.

G. Karwasz: Known and unknown in electron-atom and molecule scattering

Prof Karwasz outlined the status of data from experiments, theories, semi-empirical methods and existing databases using recent work on electron-CH_4 as an exemplary case. Elastic cross sections are pretty well known for small targets, like CH_4 but experiments and theories lack and/or disagree on polar targets (including H_2O), and heavier targets (like C_6H_6). The level of agreement between elastic and momentum transfer cross sections is still poor for molecular targets. Re-analysis of existing swarm, cross-check of different modeling codes (two-term Boltzmann, multi-term, Monte Carlo) and new beam measurements at low energies are needed. Born approximation works pretty well for IR-active vibrational cross sections but not for Raman modes; various theories generally disagree, especially at resonances. Rotational excitation, especially on polar molecules, could be also described by Born approximation, but even for water the picture could be more complicated. Ionization cross sections (integral and differential) can be described by Born-Bethe Binary Encounter Model (BEB), and agrees well with experiments. For *partial* ionization cross sections, work is in progress. Electronic excitation cross sections present the biggest challenge: recent calculations in CH_4 agree with experiments on dissociation cross sections but direct electronic excitation measurements seem unreliable.

V. Kokoouline: Uncertainty evaluation in theoretical calculations of cross sections and rate coefficients

Prof Kokoouline described a systematic approach to evaluate uncertainties in theoretical determination of cross sections in two-body collisions, such as electron-molecule collisions. There are several advantages of the Unified Monte-Carlo approach developed in nuclear physics: (1) It allows one to evaluate the uncertainty of final theoretical cross sections, if uncertainties of all parameters