Inelastic squared form factors of the valence-shell excitations of hydrogen studied by high-energy electron scattering

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Synopsis Utilizing the high-energy electron scattering technique at 1500 eV, absolute inelastic squared form factors of four vibronic series belonging to the $B^1\Sigma_u^+$, $C^1\Pi_u$, $EF^1\Sigma_g^+$ and $B'^1\Sigma_u^+$ electronic states of molecular hydrogen have been determined experimentally. In addition, the same inelastic squared form factors have been calculated by the multi-reference configuration-interaction (MRCI) method for the $B^1\Sigma_u^+$, $C^1\Pi_u$, and $EF^1\Sigma_g^+$.

The electronic structures of the excited states of atoms and molecules can be described by the inelastic squared form factors (ISFFs), which are directly related to the wave functions of the ground and excited states in the momentum space. High-precision experimental ISFFs can test the theoretical calculations strictly. The ISFFs of H_2 have been studied by high energy electron energy loss spectroscopy (EELS) experimentally. However, for the ISFFs measurement, only the spectra with electronic states resolved can be found in the literatures. Recently, we carried out a high-energy vibronically resolved electron scattering measurement of valence shell excitations of H_2 at 1500 eV. In addition, the same inelastic squared form factors are calculated by the MRCI method for the $B^1\Sigma_u^+$, $C^1\Pi_u$, and $EF^1\Sigma_g^+$. A typical spectrum of H_2 at the scattering angle of 1.5° is shown in Fig.1.

At present, the data analysis are still in progress. As a primary result, the present ISFFs of $B^1\Sigma_u^+$ (v'=0-5) of H_2 are shown in Fig. 2 along with the present calculations. The ISFFs calculated by Kolos *et al* [1] and Borges *et al* [2] are also plotted in Fig 2. These two theoretical calculations studied vibronic excitations without using of Franck-Condon principle. It is obvious that the calculated results and the present EELS ones have the similar shape, and the theoretical ISFFs fit the experimental results better in the high momentum transfer region. However, in the low momentum transfer region, both theoretical results are smaller than the experiment results. Similar phenomena have been observed for the higher vibrionic excitations. To elucidate this phenomena, more elaborate theoretically investigations are greatly recommended.

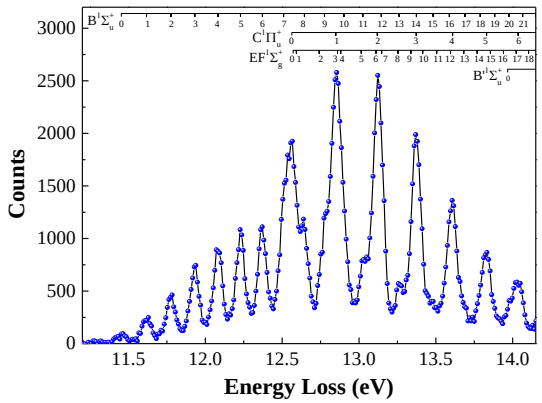

Figure 1. A typical spectrum of H_2 at the scattering angle of 1.5°.

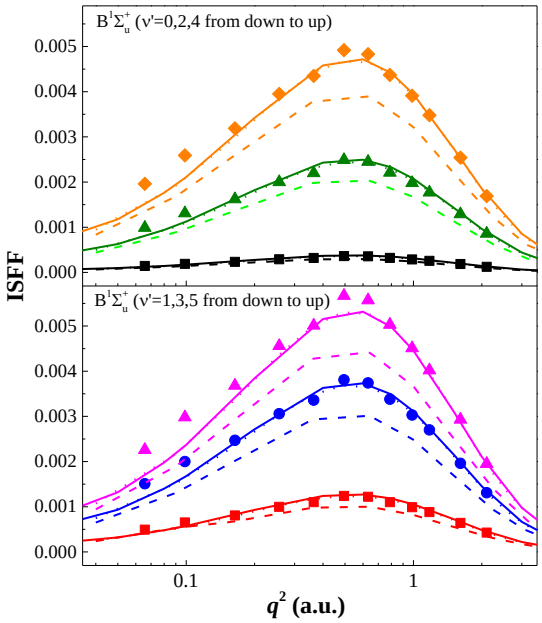

Figure 2. The ISFFs of the vibronic excitations of hydrogen. Solid points: the present EELS results; solid lines: the present MRCI calculations; dash lines: the results calculated by Borges; dot lines: the results calculated by Kolos; different colors represent different vibrionic states.

References

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[2] I. Jr. Broges and C. E. Bielschowsky, 1999 *Phys. Rev. A.* **60** 1226

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