Inelastic squared form factors of the valence-shell excitations of hydrogen studied by high-resolution inelastic x-ray scattering

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Synopsis Utilizing the high-resolution inelastic x-ray scattering technique, 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 are determined experimentally. In addition, the same inelastic squared form factors are calculated by the multi-reference single and double-excitation configuration-interaction method for the $B^1\Sigma_u^+$, $C^1\Pi_u$, $EF^1\Sigma_g^+$. Apparent differences are observed between the present experimental results and all available calculated ones.

The electronic structures of the excited states of atoms and molecules can be described by the so-called inelastic squared form factors (ISFFs). The ISFFs are directly related to the wave functions of the ground and excited states in the momentum space, and can be used to test the theoretical calculations strictly. The ISFFs of H_2 have been studied by high energy electron energy loss spectroscopy (EELS) experimentally, and only electronic states resolved spectra can be found in the literatures. Moreover, some recent investigations found that the higher Born term can not be ignored in the high-energy electron impact process, especially at large momentum transfer. To avoid the effect of higher order terms, the inelastic x-ray scattering (IXS) method was applied to study the excitation of atoms and molecules lately [1]. The results of IXS have been proven to be accurate and thus can serve as the benchmark data. So we carried out a vibronically resolved IXS measurement of valence shell excitations of H_2 at BL12XU of Spring-8.

As an example, the present ISFFs of $B^1\Sigma_u^+$ (v'=9) and $C^1\Pi_u$ (v'=6) of H_2 are shown in Fig.1 along with the calculated results by Kolos et al[2] and Borges et al[3]. These two theoretical calculations studied vibronic excitations without using of Franck-Condon principle. It is obvious in the figure that the calculated results and the present IXS ones have the similar shape, and the theoretical ISFFs fit the experimental result 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 other excitations. To elucidate them, more elaborate theoretically investigations are greatly recommended.

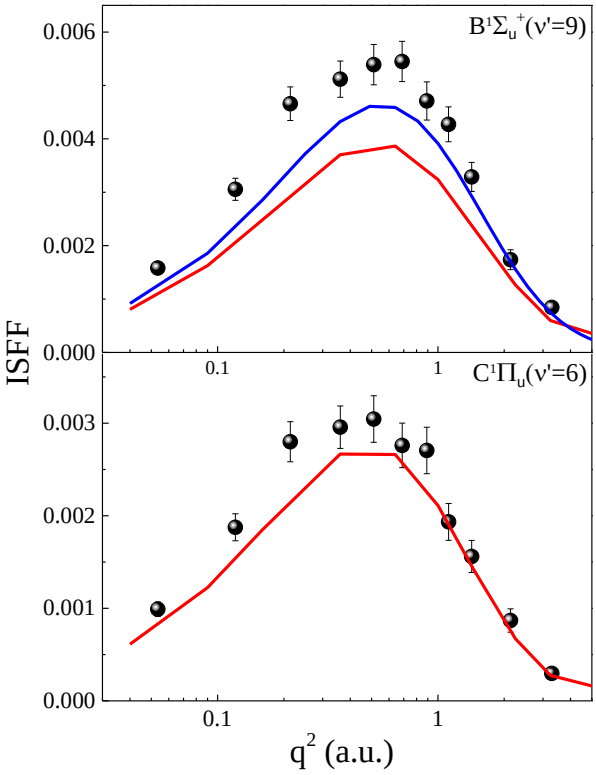

Figure 1. The ISFFs of the vibronic excitation of hydrogen. Solid black points: the present IXS results; solid red lines: the results of Borges et al; solid blue lines: the results of Kolos et al.

References

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