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# Improved nonlocal resonance model for electron - HCl collisions

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**Synopsis** We present an improved nonlocal resonance model for electron-HCl collisions. The short-range part of the model is based on *ab-initio* electron scattering eigenphase sums calculated using the Schwinger Multichannel method and the long-range part on the potential curve of the bound $HCl^-$ anion. We have calculated cross sections for vibrational excitation and dissociative electron attachment. For all collision processes where quantitative experimental data are available, the new model agrees with experiments better than the previous model.

Hydrogen chloride constitutes an ideal system for testing theoretical models for electron-molecule collisions because of the wide variety of phenomena seen in the cross sections. The so-called nonlocal resonance model [1] has so far provided the most complete qualitative description of the resonance and threshold features observed in low-energy electron-HCl collisions. However, recent measurements of dissociative electron attachment (DEA) cross sections [2] showed that the model of Ref. [1] (further referred to as the DMHC model) overestimates the DEA cross section by approximately a factor of 2.5, and it has been suggested that the reason for this discrepancy lies in the old *ab-initio* electron-HCl scattering data that were used in constructing the DMHC model.

We present an improvement of the DMHC model via modification of the short-range part of ion potential involved in the model. The new short-range part has been fitted on the electron scattering eigenphase sums calculated using the Schwinger Multichannel method. Other components of the nonlocal resonant model — potential curve of the neutral HCl and long-range potential curve of the bound $HCl^-$ anion — were kept the same as in the DMHC model.

Table 1 shows the comparison of the energy integrated DEA cross sections for HCl and DCl with the recent experimental data [2]. The present model agrees much better with experimental data than the DMHC model.

The present model also partly resolves an old controversy in the DEA temperature dependence in HCl. Figure 1 compares the predicted temperature effect on DEA with that observed by of Allan and Wong [3]. The agreement with the experiment is better in the present model. Additionally, the present model reproduces all qualitative structures observed in the elastic scattering and vibrational excitation cross sections.

**Tab. 1**. Integrated DEA cross sections in eVÅ$^2$.

| | New model | DMHC model [1] | Exp. [2] |
|---|---|---|---|
| HCl | $6.14\times10^{-2}$ | $14.90\times10^{-2}$ | $6.85\times10^{-2}$ |
| DCl | $0.28\times10^{-2}$ | $1.25\times10^{-2}$ | $0.45\times10^{-2}$ |

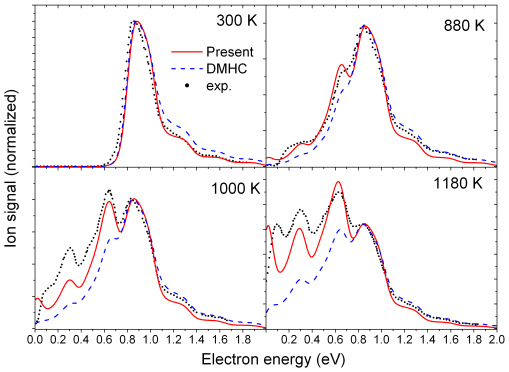


**Fig. 1**. DEA temperature dependence. Solid line: present model; dashed line: DMHC model [1]; points: experimental data by Allan and Wong [3].

## References

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