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# MULTIPLE IONIZATION CROSS SECTIONS BY ION IMPACT ON Ne-like MOLECULES

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## Abstract

Single and **Multiple Ionization Cross Sections (MICS)** by ion impact on Ne and Ne-like molecules are calculated in the framework of the **Independent Electron Model (IEM)** and taken into account post-collisional effects like Auger and Coster-Kronig processes. The single particle probabilities in the MICS, are represented by decreasing exponential functions, called the **Exponential Model (EM)**. The net ionization cross sections by atomic or molecular orbital required as input by the EM, are calculated using the **CDW-EIS** approximation. The MICS calculated with the EM probabilities are in very good agreement with experimental data and present better agreement than other more complex theoretical models

## Theoretical Model

### Independent Electron Model

The collision is seen as a product of independent interactions between the projectile and the target electrons. Electron correlation is not considered

### Q-fold Ionization Cross Section

$$\sigma_q = 2\pi \int b P_q(b) db$$

$$P_q(b) = \sum_{q_1+q_2+q_3+\alpha=q} \prod_{i=1}^3 \binom{N_i}{q_i} p_i^{q_i} (1-p_i)^{N_i-q_i} \mathcal{P}(q_1, q_2, q_3, \alpha)$$

Post-collisional correction

$$\mathcal{P}(q_1, q_2, q_3, \alpha) = \sum_{\alpha_j=0}^{\alpha} \prod_{j=1}^{q_1} m_{1s}(q_2, q_3, \alpha_j) \prod_{j=q_1+1}^{q_1+q_2} m_{2s}(q_3, \alpha_j)$$

Ne post-collisional Auger Probabilities

$$m_{1s}(q_2, q_3, \alpha) = \begin{cases} 1 - \frac{8-q_2-q_3}{8} (1-\beta_{1s}(\alpha)) & \alpha=0 \\ \frac{8-q_2-q_3}{8} \beta_{1s}(\alpha) & \alpha \neq 0 \end{cases}$$

$$m_{2s}(q_3, \alpha) = \begin{cases} 1 - \frac{6-q_3}{6} (1-\beta_{2s}(\alpha)) & \alpha=0 \\ \frac{6-q_3}{6} \beta_{2s}(\alpha) & \alpha \neq 0 \end{cases}$$

$\alpha$	$\beta_{1s}(\alpha)$	$\beta_{2s}(\alpha)$
0	0.010	0.873
1	0.736	0.119
2	0.220	0.008
3	0.031	
4	0.003	

Carlson et al. Phys. Rev. **151** (1966) 151-47

### Exponential Model (EM): single particle probability for ionization

$$p_i(b) = p_{i0} e^{-b/r(i)}$$

$$r(i) = \frac{n_i^2}{\sqrt{-2n_i^2 \epsilon_i}}$$

The parameter  $p_{i0}$  needs to reproduce *CDW-EIS* total cross sections for single-electron emission per electron for each orbital

### Ne

Atomic Orbital	Populations	Binding energy (eV)
1s	2	-891,4
2s	2	-52,5
2p	6	-23,13

### CH<sub>4</sub>

Molecular Orbital	Populations	Binding energy (eV)
C1s (2)	2.00 C1s	-290.7
2a <sub>1</sub> (2)	1.133 C2s + 0.867 H1s	-22.9
1t <sub>2</sub> (6)	3.399 C2p + 2.601 H1s	-12.6

### NH<sub>3</sub>

Molecular Orbital	Populations	Binding energy (eV)
1a <sub>1</sub> (2)	2.00 N1s	-405,6
2a <sub>1</sub> (2)	1.207 N2s + 0.067 N2p + 0.726 H1s	-31.13
1e (4)	2.31 N2p + 1.69 H1s	-17.19
3a <sub>1</sub> (2)	0.238 N2s + 1.719 N2p + 0.043 H1s	-10.16

## Conclusions

- Multiple Ionization Cross Sections of Ne, H<sub>2</sub>O, NH<sub>3</sub> and CH<sub>4</sub> by ion impact were obtained applying the Independent Electron Model and taken into account post-collisional effects.
- The results obtained using EM single particle probabilities + post-collisional effects are in very good agreement with experimental data.
- Post-collisional effects dominates the Double Ionization Cross Sections for energies higher than 1 MeV for proton impact, but it depends on the ionization degree.
- We will continue investigating the applicability of the EM-MICS model to describe the fragmentation channels of Ne-like molecular targets.

## Acknowledgements

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## Ne, CH<sub>4</sub>, NH<sub>3</sub> and H<sub>2</sub>O

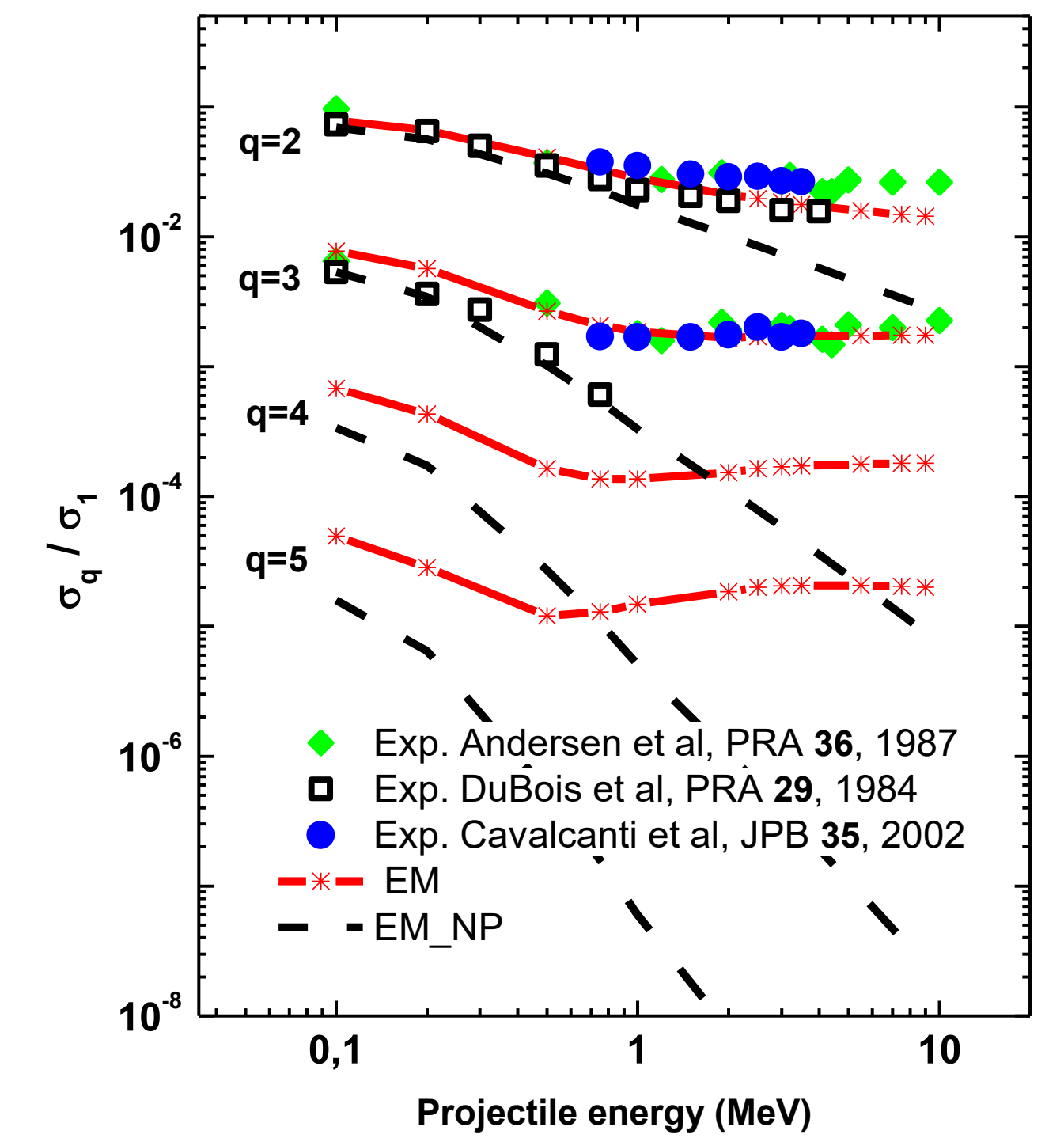
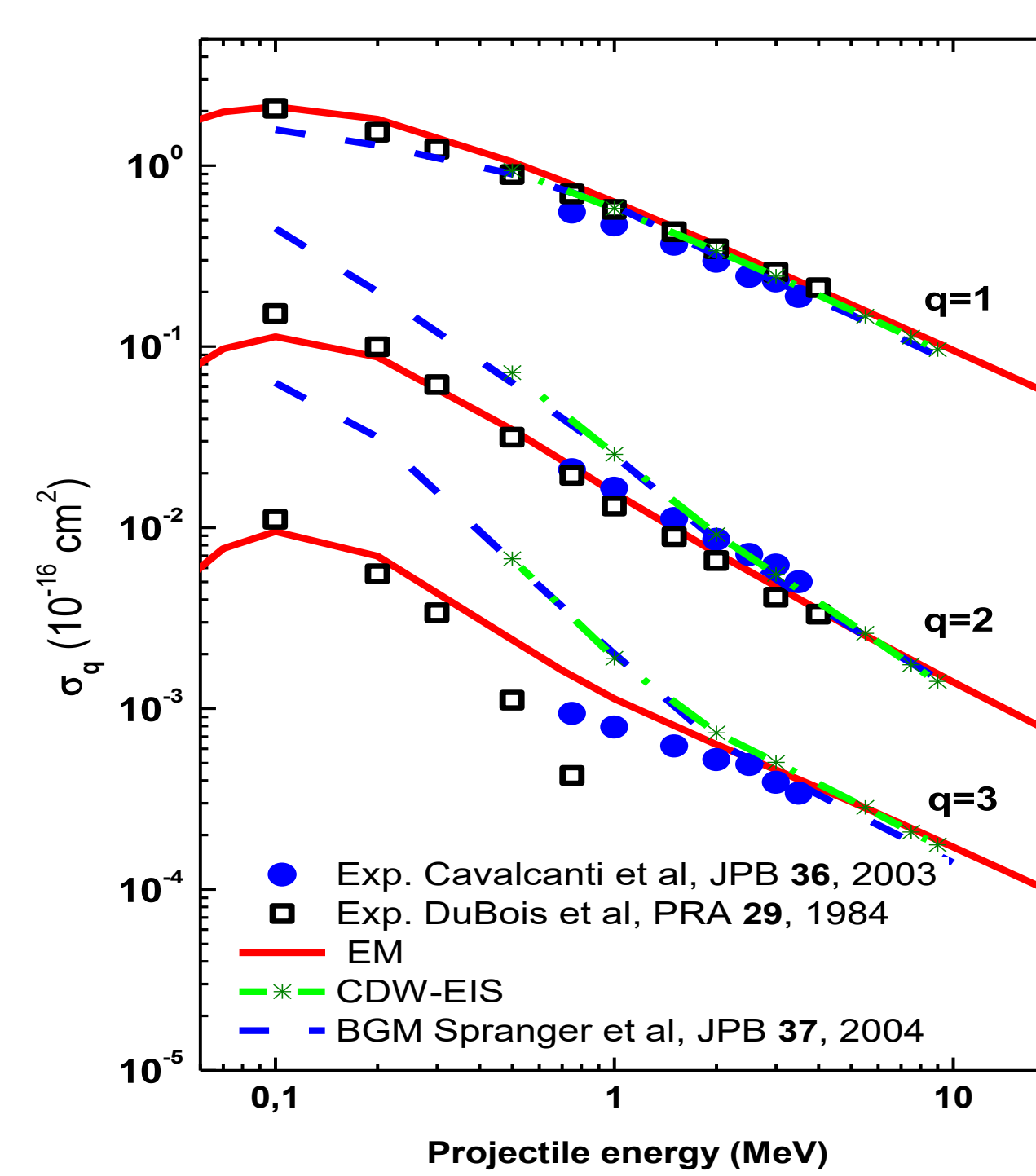
### Processes for target electron loss:

- Single and multiple Ionization
- Electron capture ⇒ Not considered in this work
- Auger-like ionization processes ⇒ Very important at high projectile energy!

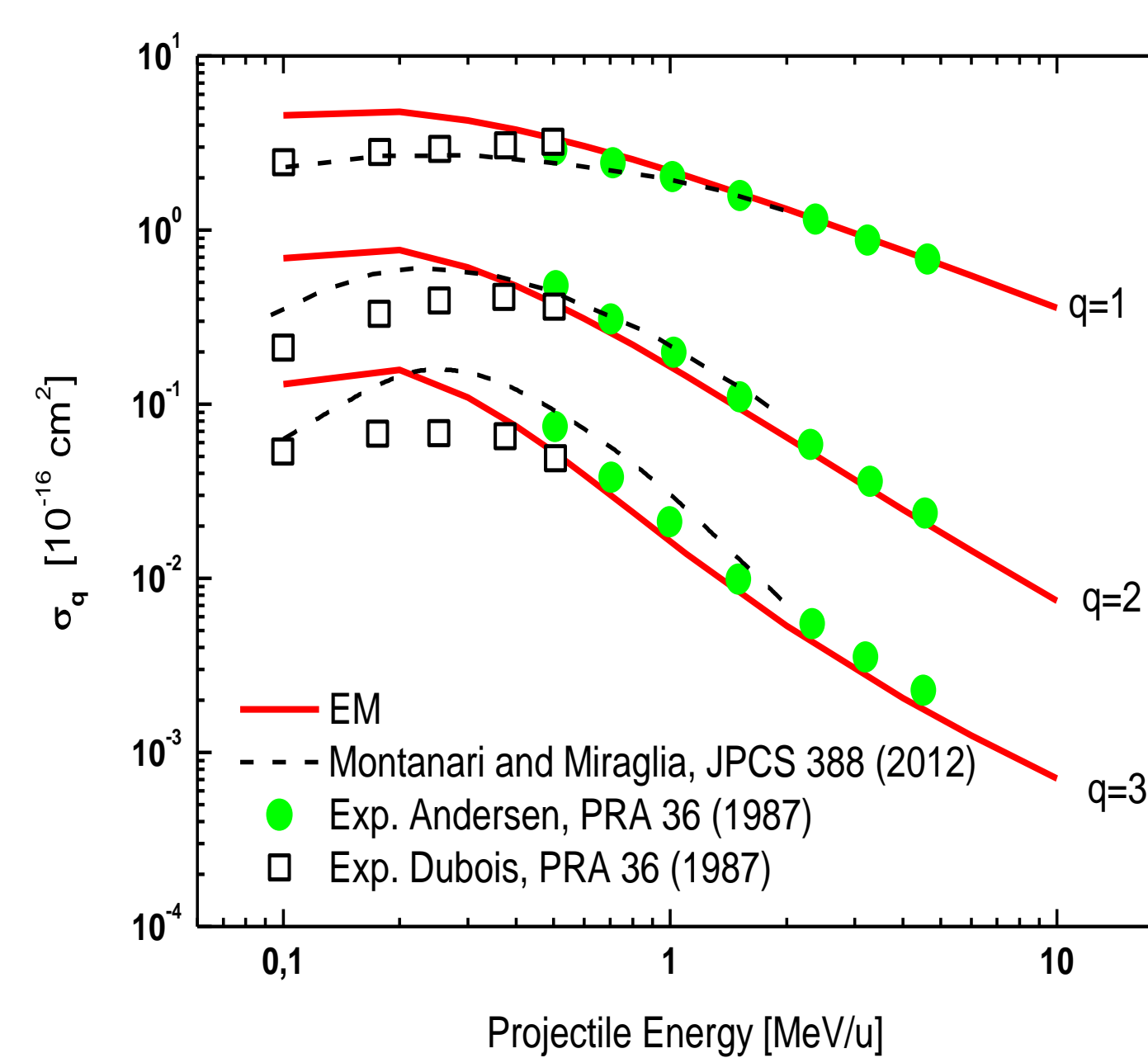
## Multiple ionization Cross Sections

### H<sup>+</sup> + Ne

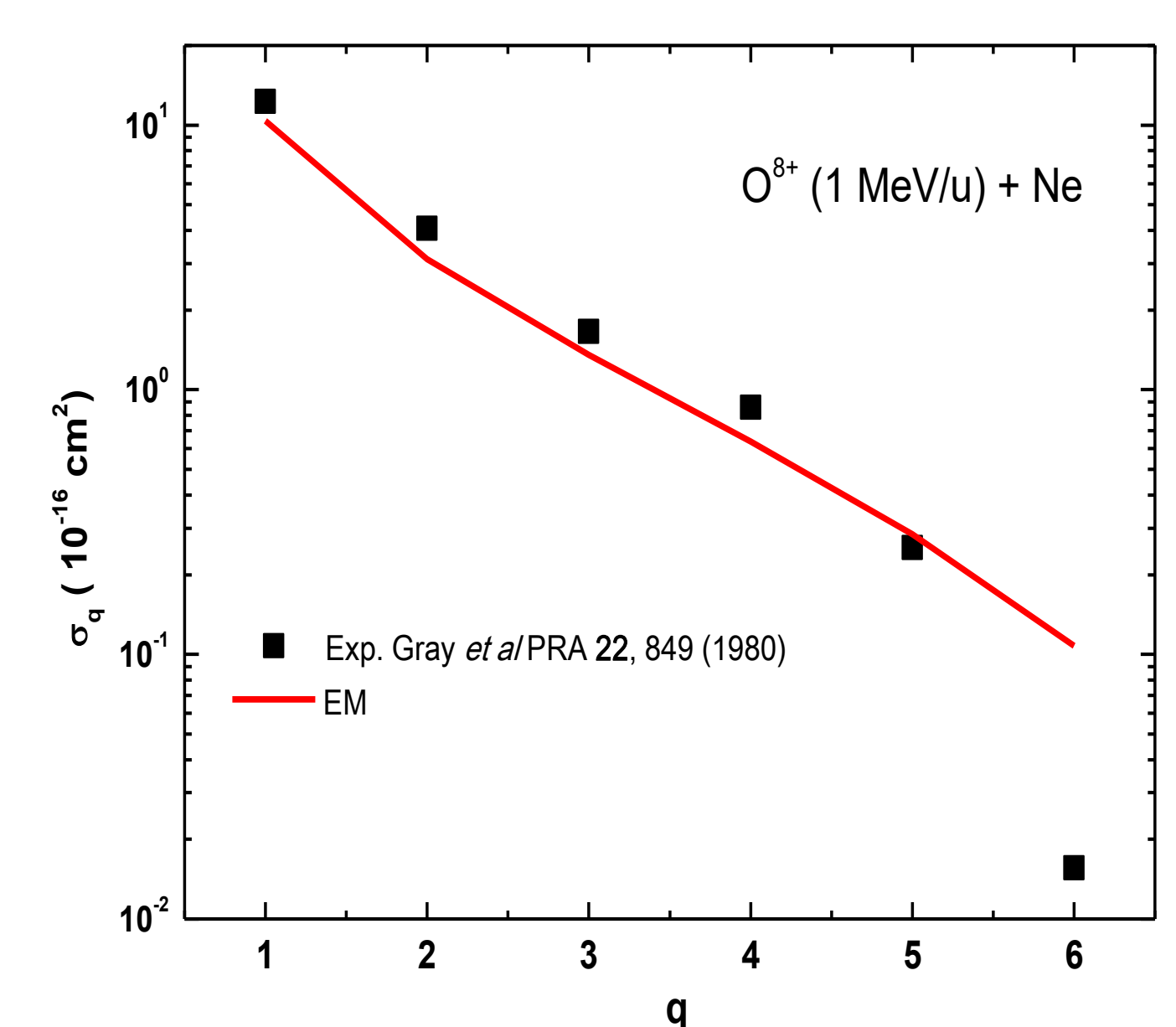
Galassi M E, Rivarola R D, and Fainstein P D 2007 Phys. Rev. A 75 052708



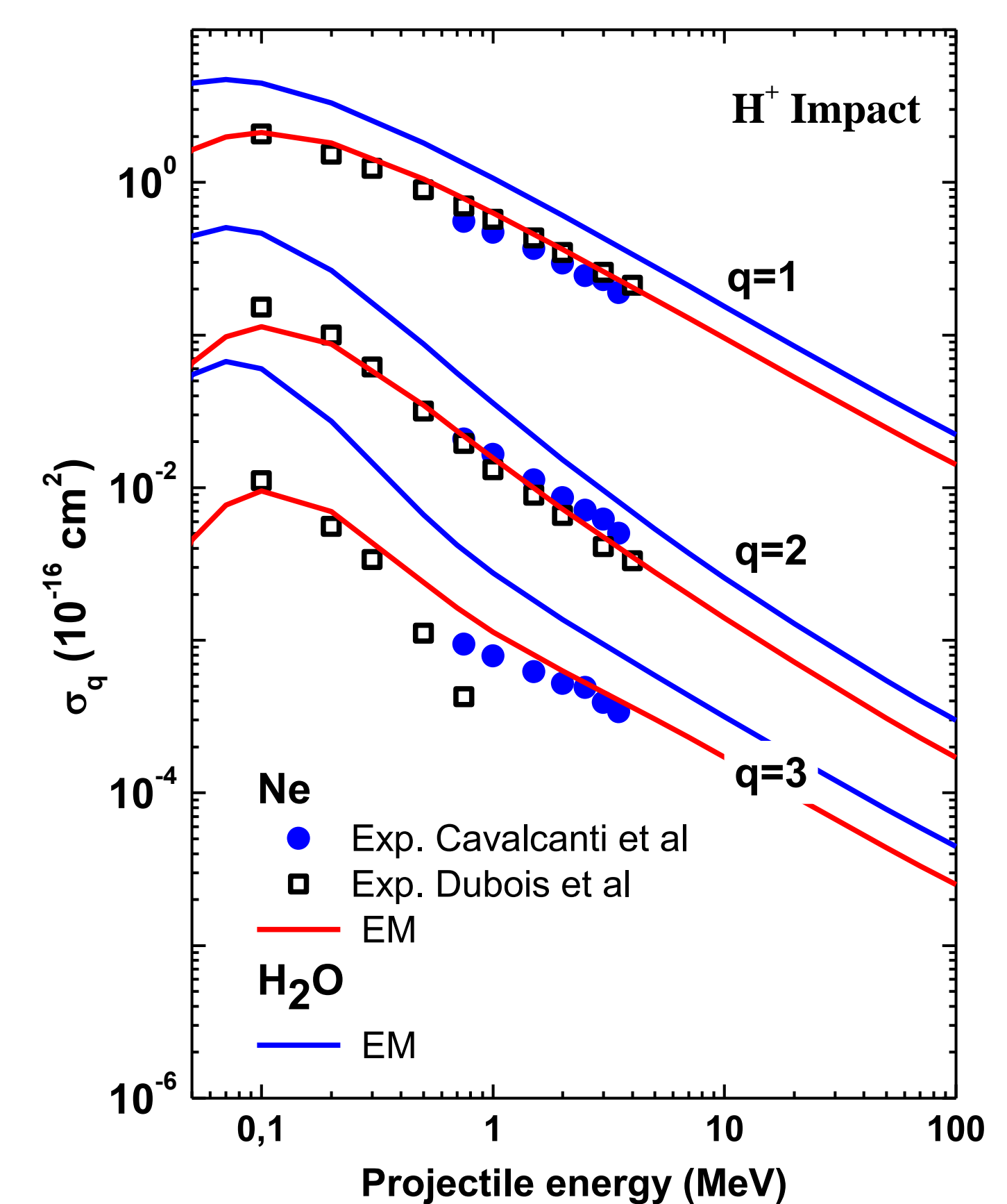
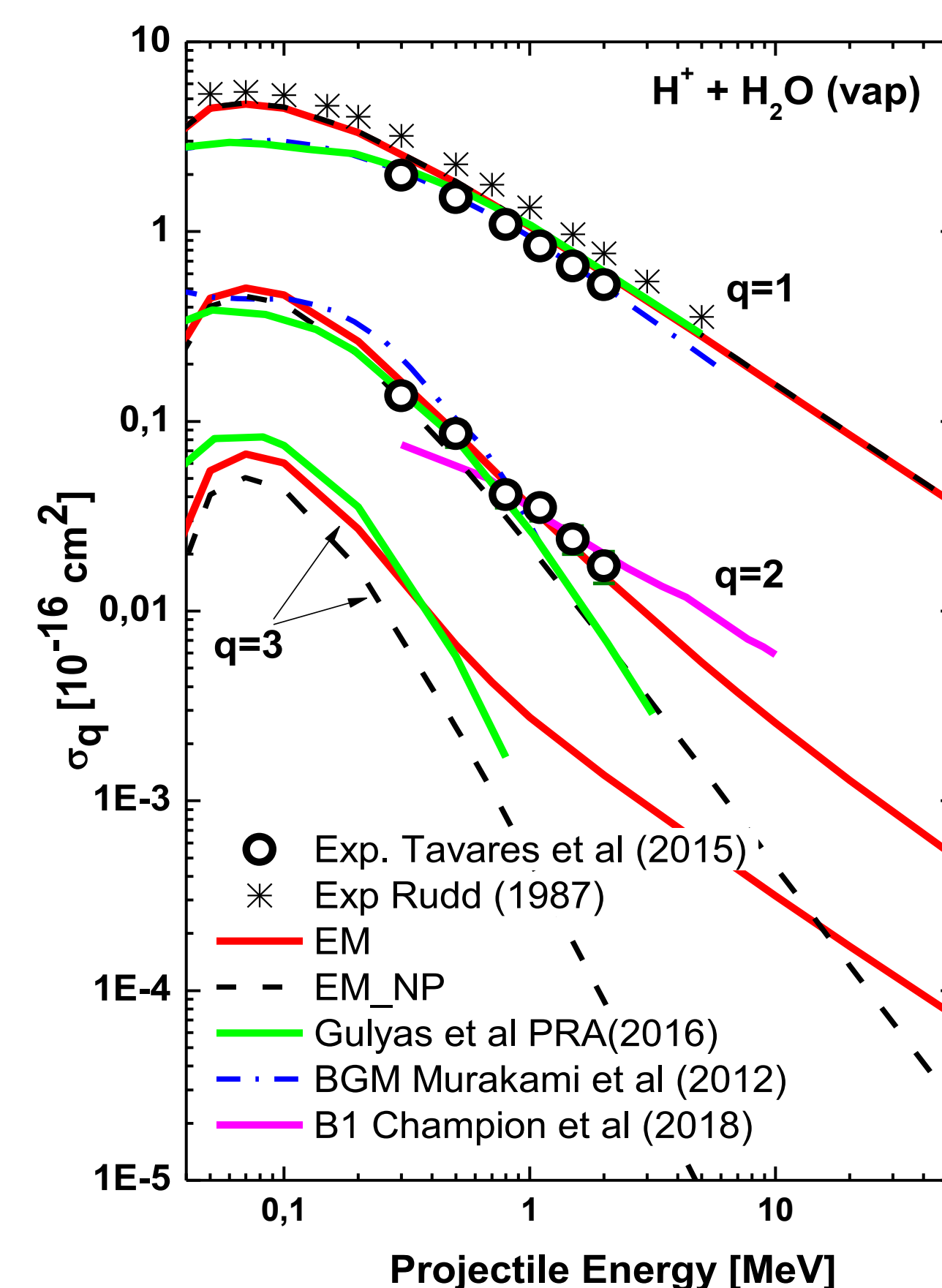
### He<sup>2+</sup> + Ne



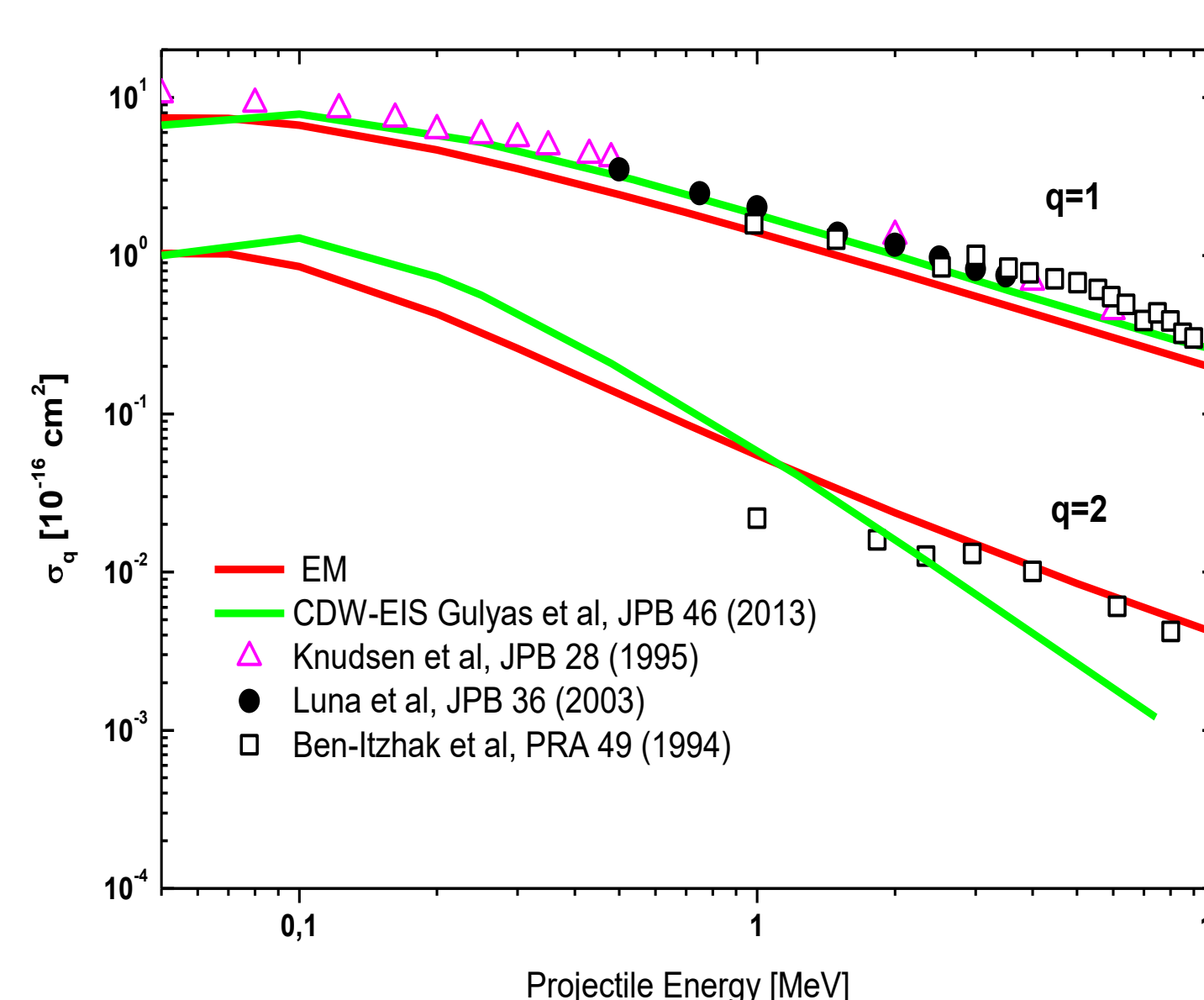
### O<sup>8+</sup> + Ne



### H<sup>+</sup> + H<sub>2</sub>O



### H<sup>+</sup> + CH<sub>4</sub>



### H<sup>+</sup> + NH<sub>3</sub>

