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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

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

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

α	$\beta_{1s}(\alpha)$	$\beta_{2s}(\alpha)$
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

CH₄

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

NH₃

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

Conclusions

- Multiple Ionization Cross Sections of Ne, H₂O, NH₃ and CH₄ 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, CH₄, NH₃ and H₂O

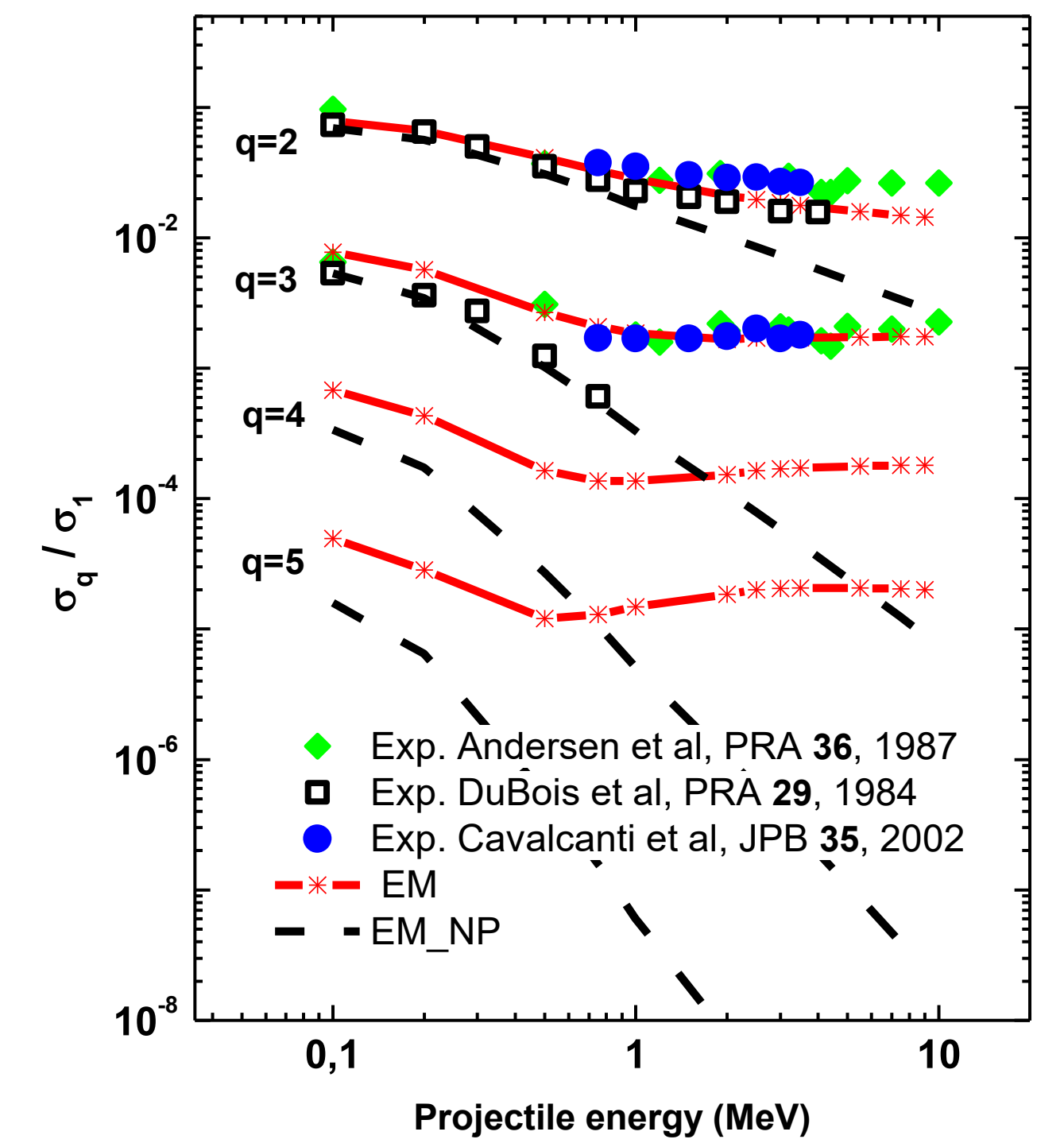
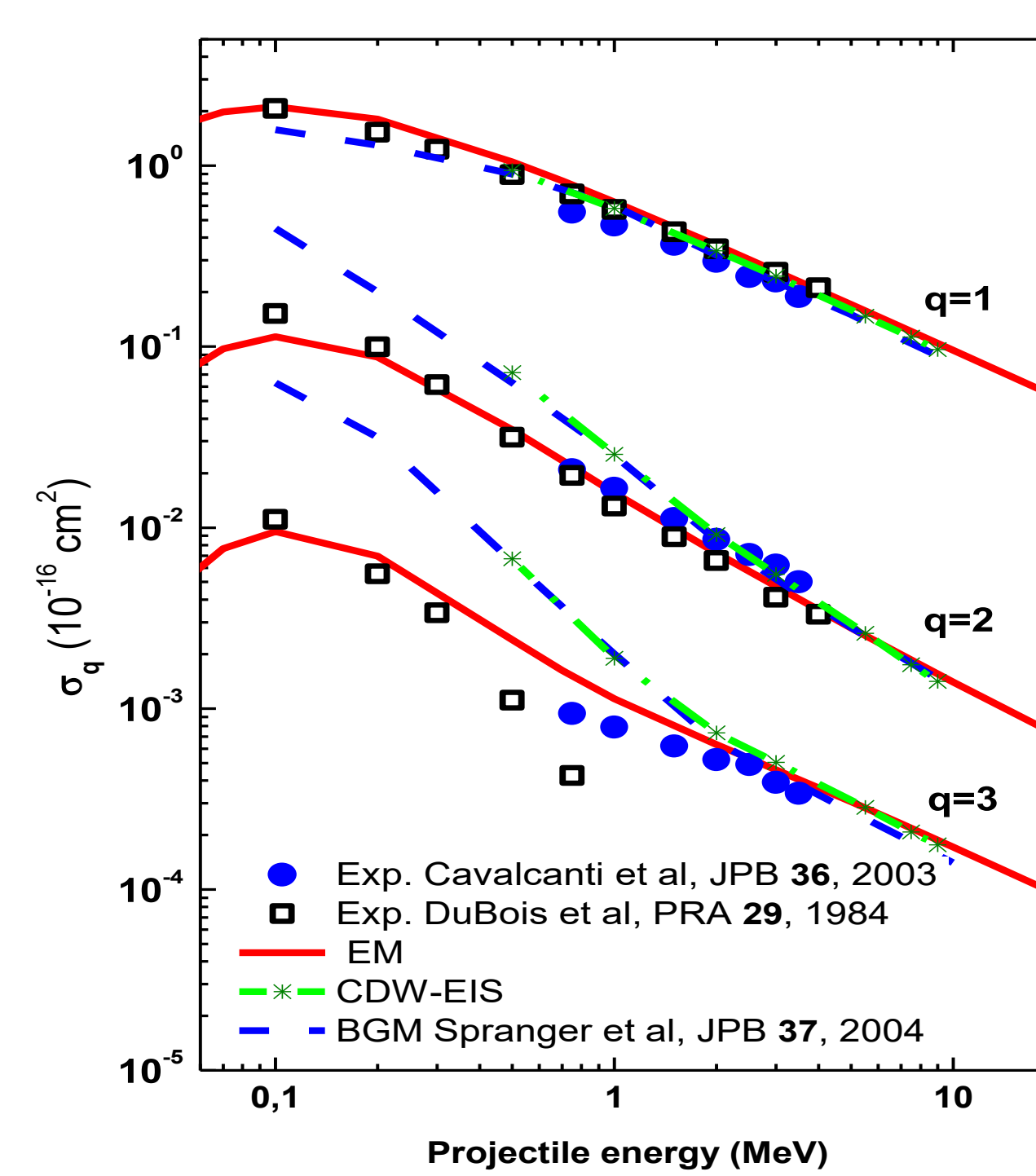
Processes for target electron loss:

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

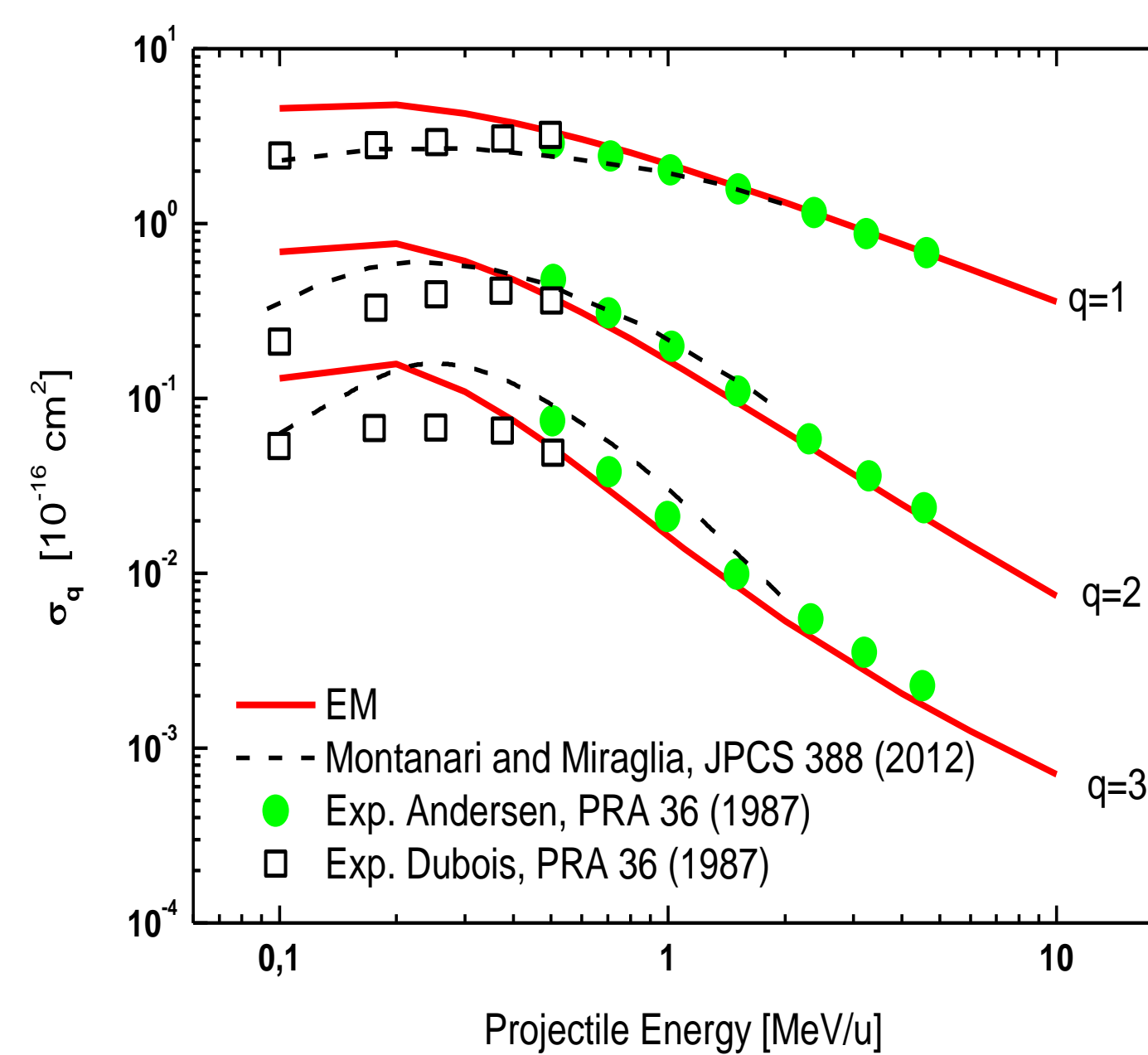
Multiple ionization Cross Sections

H⁺ + Ne

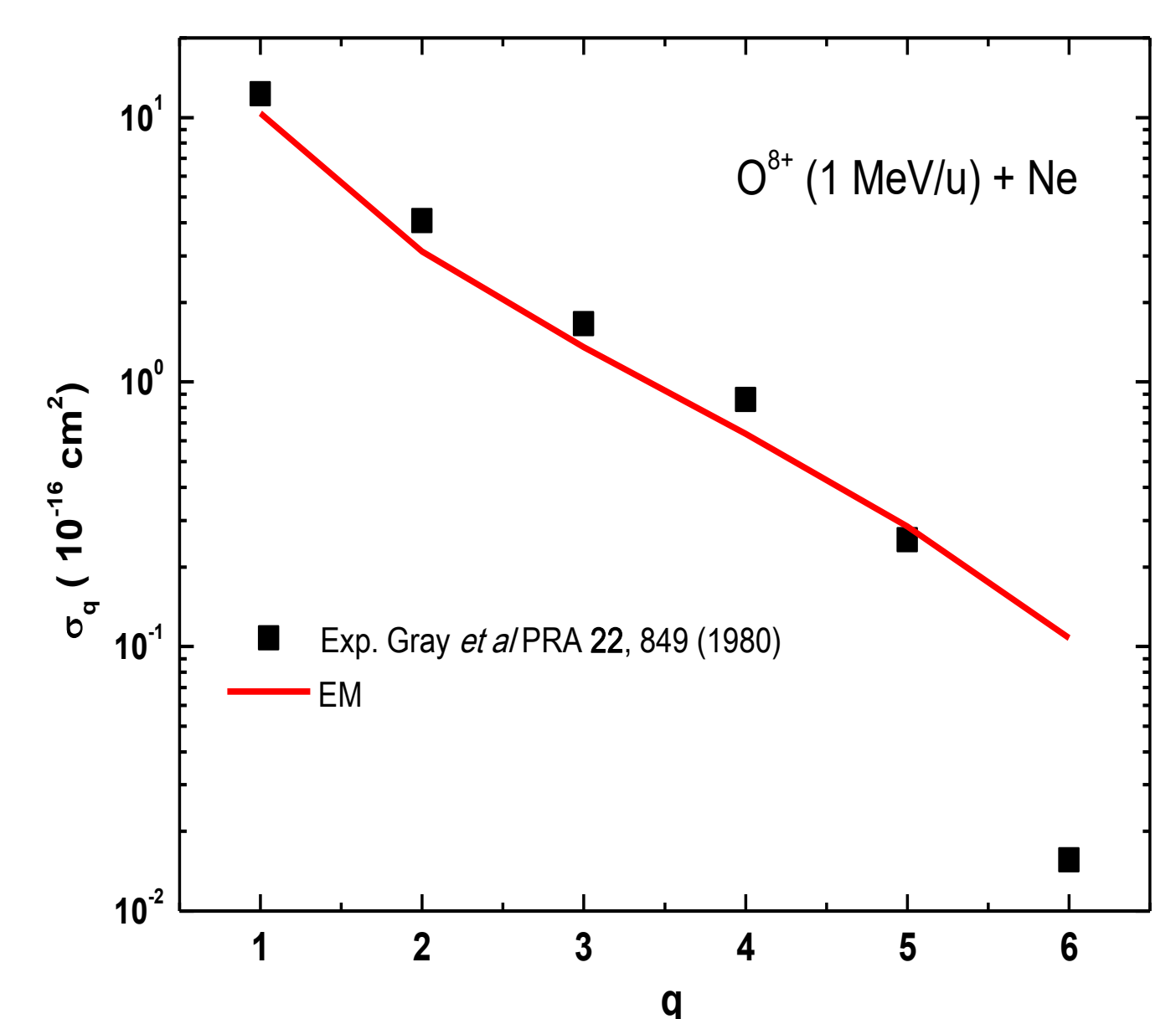
Galassi M E, Rivarola R D, and Fainstein P D 2007 Phys. Rev. A 75 052708



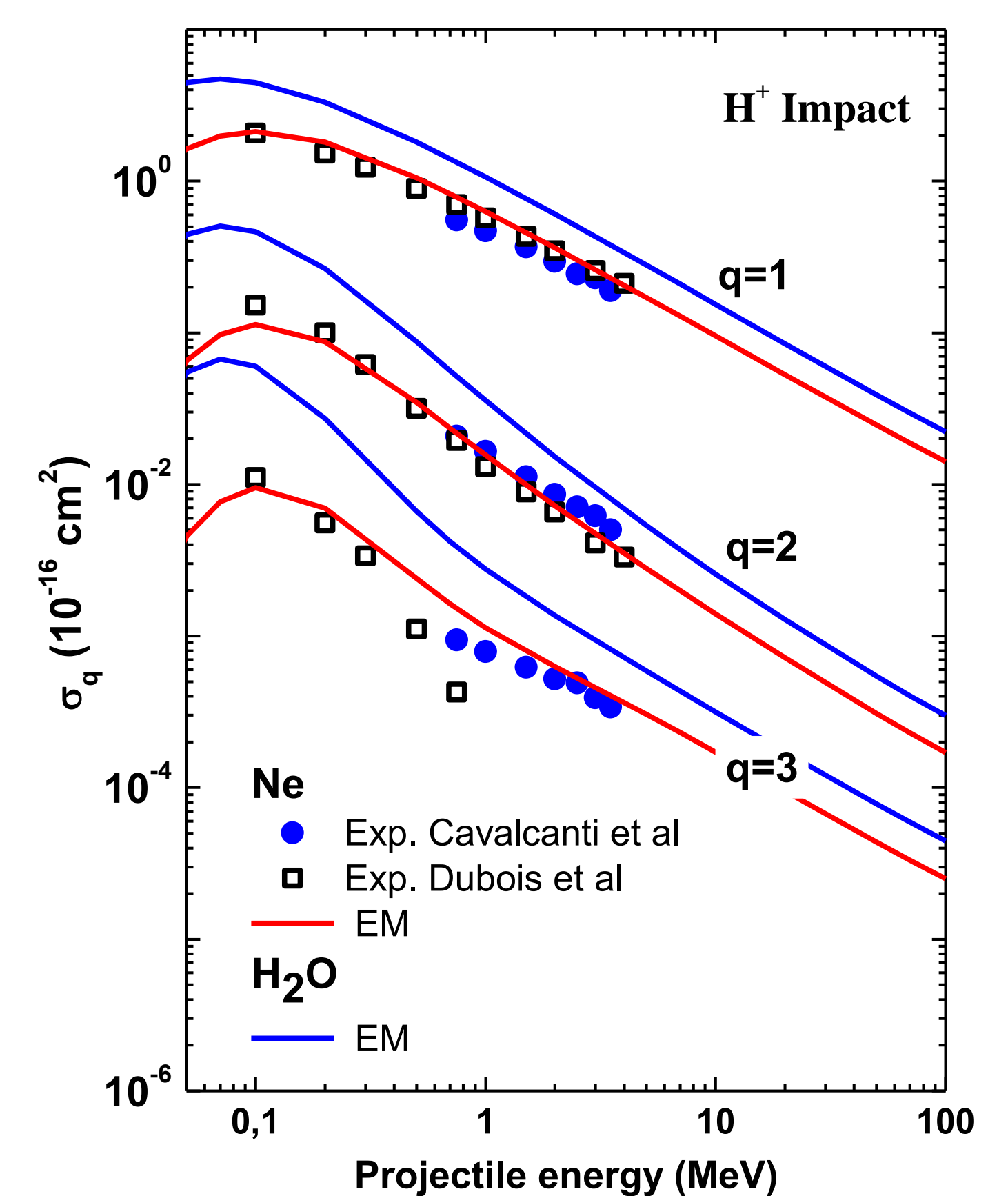
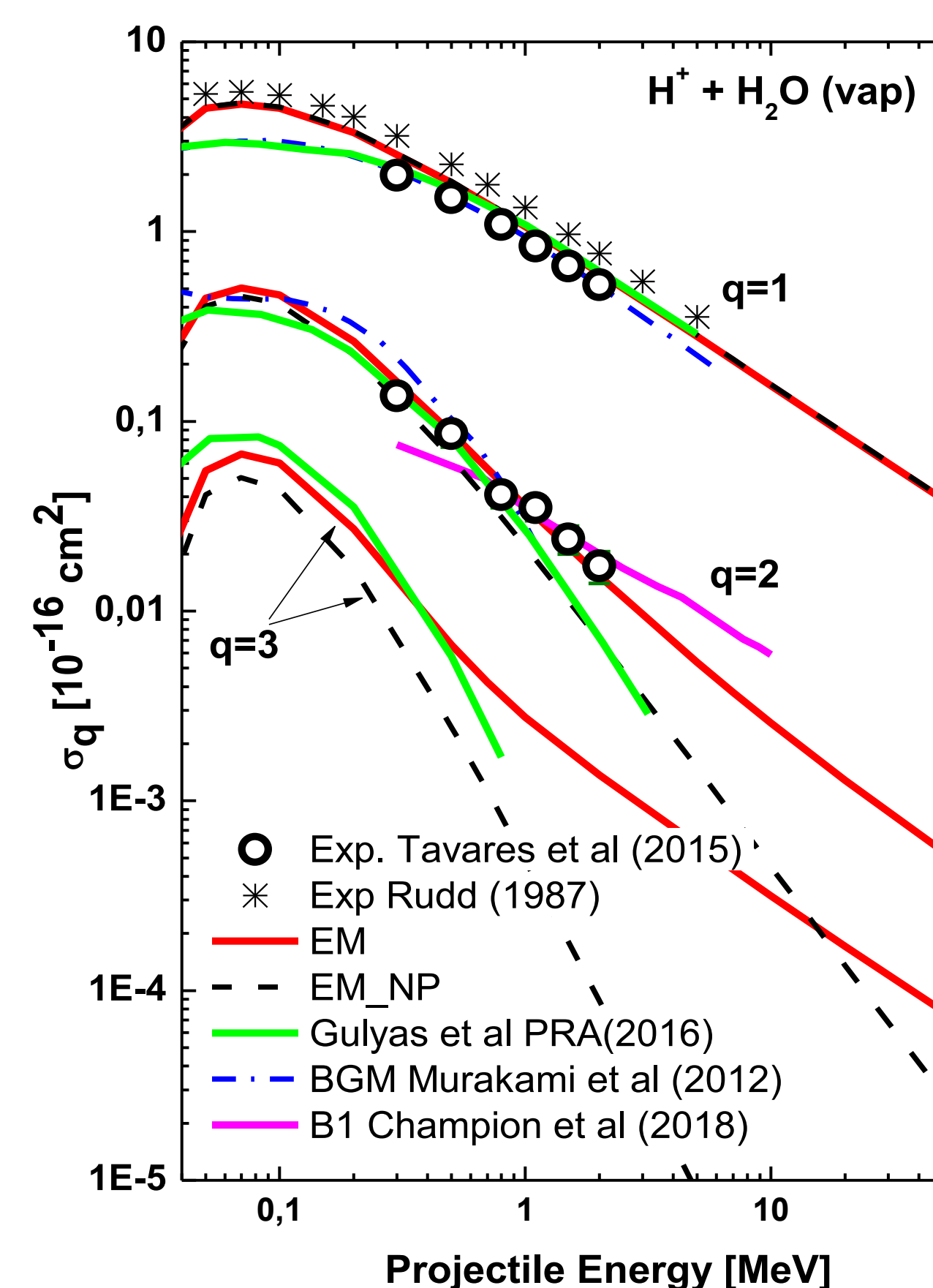
He²⁺ + Ne



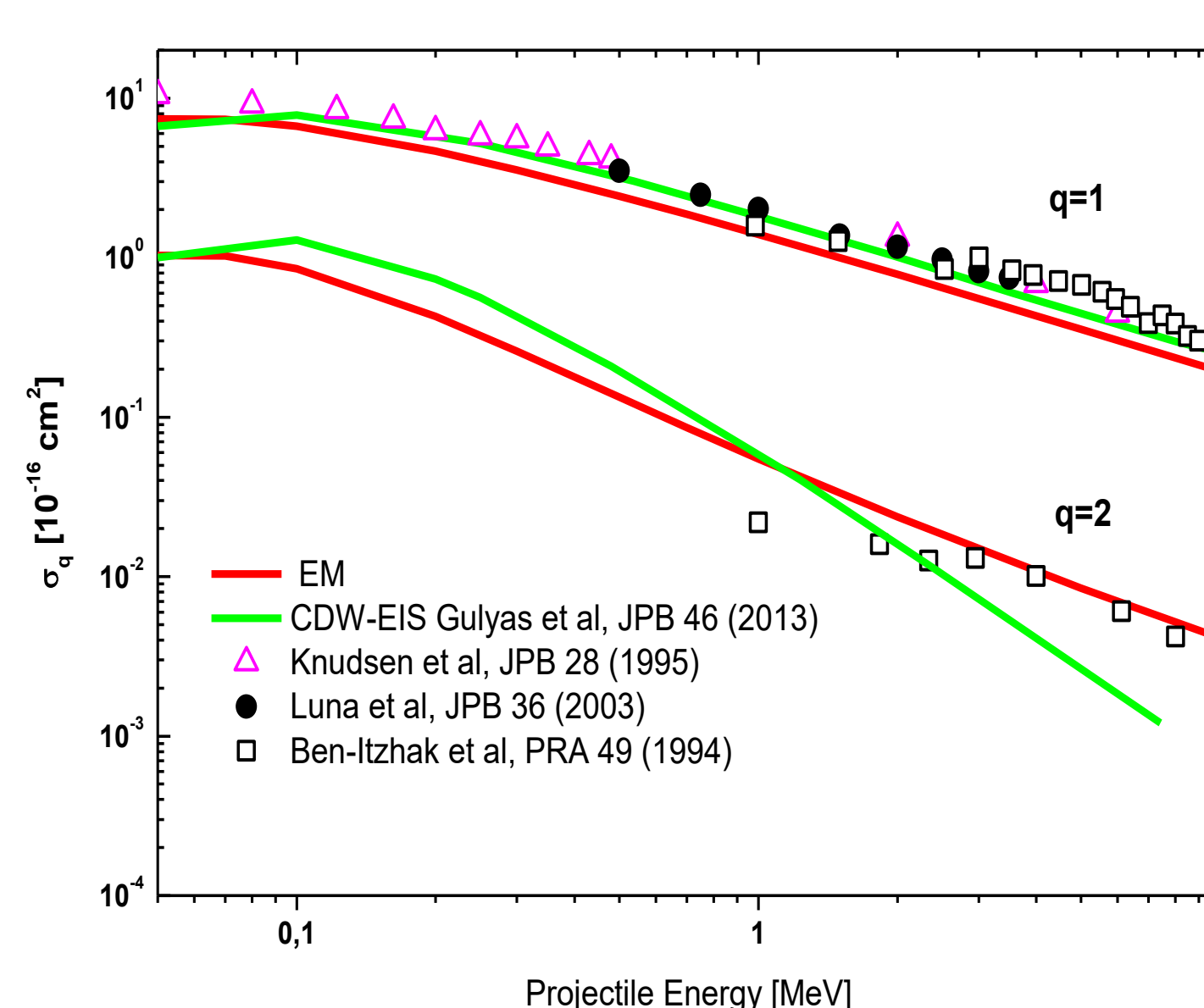
O⁸⁺ + Ne



H⁺ + H₂O



H⁺ + CH₄



H⁺ + NH₃

