Resonant photoionization of O_2 up to the fourth ionization threshold: Supporting Information

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1 Partial Photoionization Cross Section

The partial photoionization cross section into the $a^4\Pi_u$, $A^2\Pi_u$ and $b^4\Sigma_g^-$ ionic states of O_2^+ are depicted in Figures 1, 2 and 3, respectively.
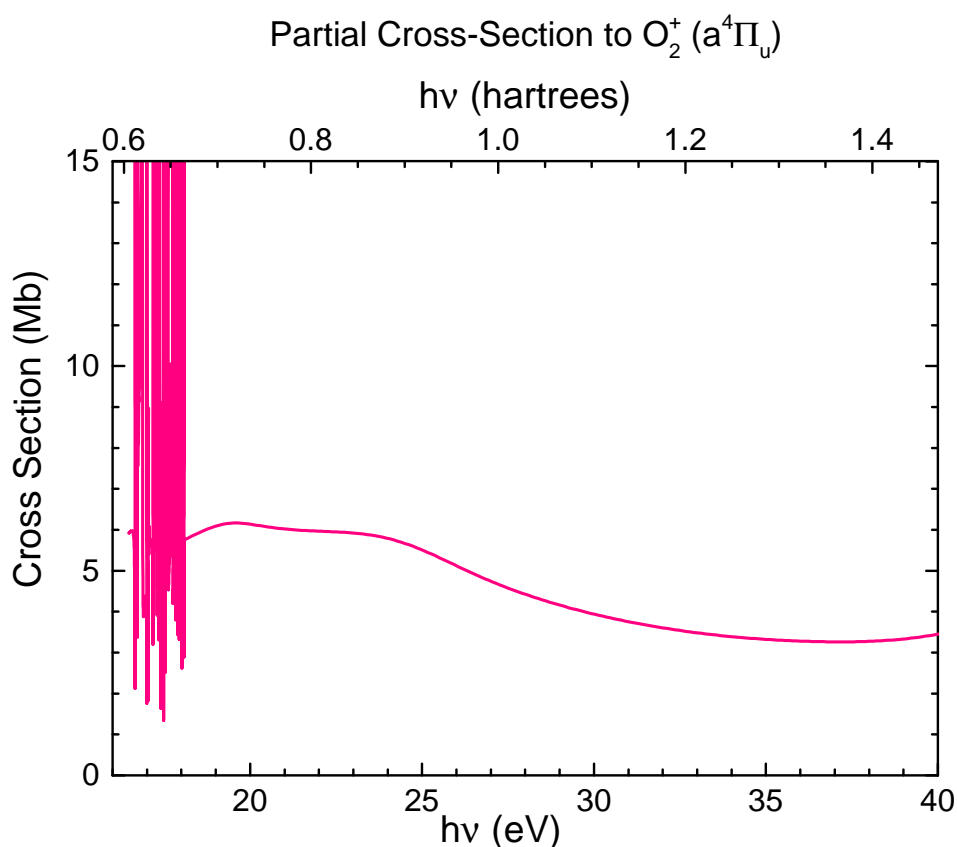

Figure 1: Computed Partial Cross section into O_2^+ ($a^4\Pi_u$).

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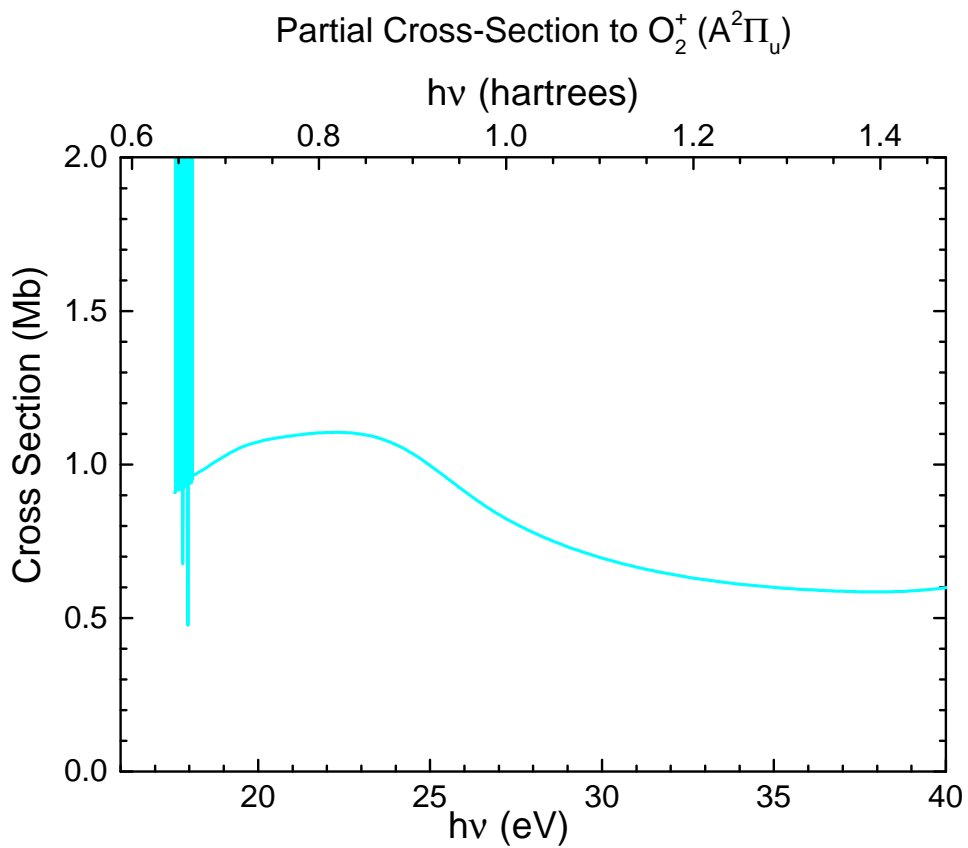[c] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain.

Partial Cross-Section to O$_2^+$ (A$^2\Pi_u$)

hν (hartrees)

Figure 2: Computed Partial Cross section into O$_2^+$ (A$^2\Pi_u$).

Partial Cross-Section to O$_2^+$ (b$^4\Sigma_g^-$)
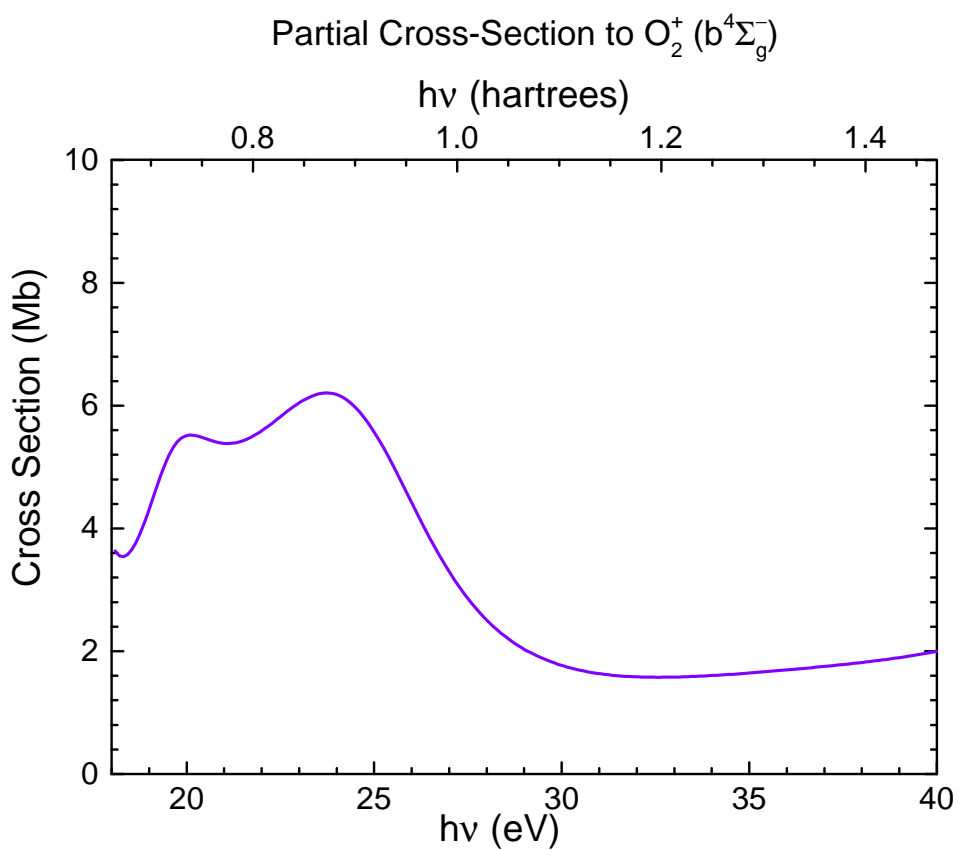
hν (hartrees)

Figure 3: Computed Partial Cross section into O$_2^+$ (b$^4\Sigma_g^-$).

2 Total Photoionization Cross Sections

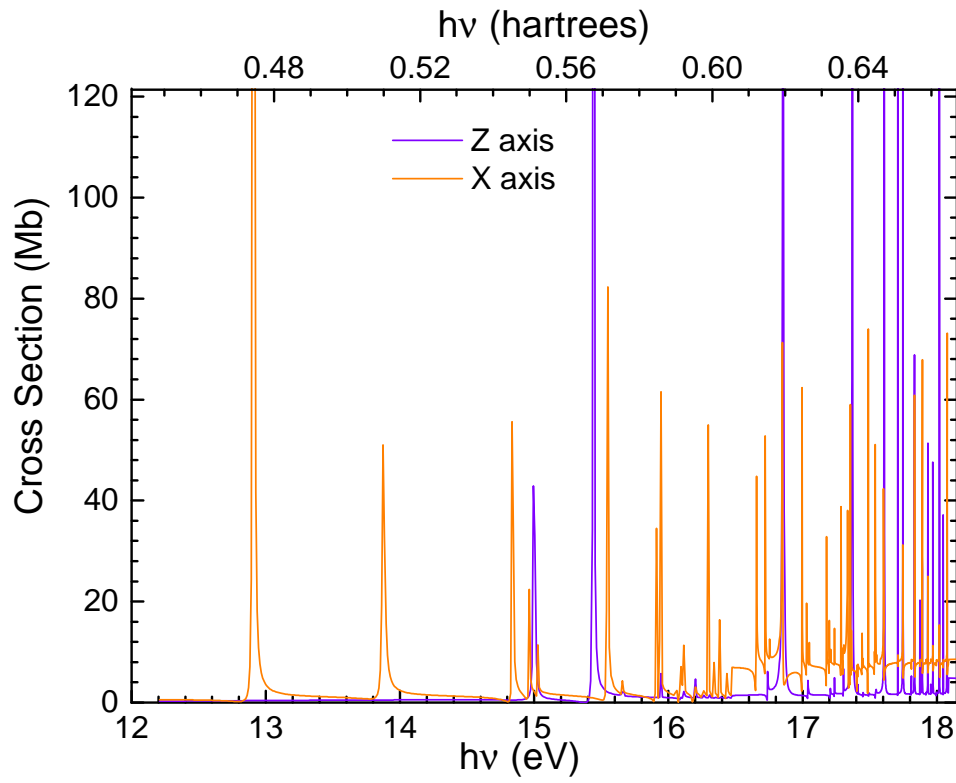The computed total photoionization cross section for the $^3\Sigma_u^-$ and $^3\Pi_u$ symmetries are shown in Fig. 4.

Figure 4: Total photoionization cross section computed for the $^3\Sigma_u^-$ (orange, labelled Z axis) and $^3\Pi_u$ (violet, labelled X axis) total symmetries.