AB INITIO STUDY OF THE H, J, I, I' AND I'' $^3\Pi_u$ SUPEREXCITED STATES OF O$_2$

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In this presentation we report progress in the computation of superexcited states of O$_2$, namely, of bound $^3\Pi_u$ Rydberg states of the neutral molecule converging to the a$^4\Pi_u$ state of O$_2^+$. Up to twenty $^3\Pi_u$ potential energy curves were computed. The MRD–CI package together with the cc–pV4Z basis set augmented with seven diffuse functions of $s$, $p$ and $d$ type on each atom were employed. This study was prompted by the demand of potential curves to try to understand the mechanism of the neutral dissociation of O$_2$ above the first ionization limit (IP= 12.07 eV) where there exists a competition between autoionization and predissociation. This undertaking focuses on the computation of the I, I’ and I'' $^3\Pi_u$ states that have been postulated as involved in the neutral dissociation of O$_2$ in the 865–790 Å (14.33–15.69 eV) energy region.