Abstract Submitted
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Suppressed and enhanced tunneling ionization of transition metal atoms and cations: a TDDFT study on nickel XI CHU, Univ of Montana — We study the tunneling ionization (TI) of Ni, Ni^+, and Ni^{2+} with a TDDFT method and reproduce the puzzling suppression of the TI of Ni and Ni^+ and the enhancement of TI in Ni^{2+}. Numerical results reveal that for all three species the electron tunnels from a $4s$ orbital, i.e., excitation precedes tunneling for both of the cations, for which the highest orbitals are $3d$. The effective radial potentials for the d orbitals have a centrifugal barrier, while there is no such barrier for the s orbitals. At the classical turning point for the $3d$ orbital, the $3d$ to $4s$ excitation energy is lower than the centrifugal potential for the d orbitals. Two factors of opposite nature are identified in this work. On one hand, electrons moving away from the nucleus in the intense laser fields induce an attractive potential that effectively lowers the energy level and thus suppresses tunneling. Excitation, on the other hand, has the opposite effect and enhances tunneling. The energy gap between $4s$ and $3d$ is small for Ni^+ and therefore suppression wins. As the charge of the cation increases, the excitation energy becomes much greater and for Ni^{2+} enhancement dominates. Based on similar analysis, we expect enhanced TI for several other cations.

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