Time-Dependent First-Principle Simulations on the Resonant High-Harmonic Generation from Transition Metal Plasma

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High-harmonic generation (HHG) as a result of interaction between atoms with high intensity laser pulses has been seen as a promising source of table-top XUV radiations. Conventionally, HH photons are produced from noble gases owing to their abundance in gas phase. However, it has been found that HHG from some transition metals can exhibit interesting features not found in HHG from noble gases.

One of such observations is the presence of enhanced harmonic peaks in the HH spectrum from some transition metal plasmas, for example in Mn plasma the enhancement occurs at 51 eV [1] and in In at 20 eV [2]. Such enhancement has been believed to be due to 3*p*-to-3*d* giant resonance. In our work we simulated HHG from Mn and Mn^+ using first-principles simulations TD-CASSCF and TD-ORMAS [4, 5, 6]. As a result, we successfully reproduce a prominent harmonic peak at around 51 eV (experimental value), enhanced several times stronger than the neighboring harmonics. Rerunning the simulation except with 3*p* orbitals frozen resulted in the disappearance of the 51 eV enhancement, which implies a critical involvement of 3*p* orbitals in the enhancement process.

In order to gain a deeper insight into the origin of the resonant enhancement in Mn and Mn^+, we also perform an analysis on the various orbital-specific quantities such as time-dependent orbital populations and orbital-orbital transition spectra using the initial orbitals with is the number of occupied orbitals. Based on this analysis, we have identified the three selection rules-obeying pair of the 3*p*-3*d* transitions to be the most important ones leading to the resonant enhancement in Mn and Mn^+. Since we employ first-principles method, the results obtained in this work are expected to provide a reliable theoretical foundation for future researches on the topic of resonant HHG.

References

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