

Abstract Submitted
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High-order harmonic generation in doped and imperfect band-gap materials¹ LARS BOJER MADSEN, CHUAN YU, KENNETH HANSEN, Aarhus University — We predict by time-dependent density functional theory simulations and rationalize by a three-step model of high-order harmonic generation (HHG) that a donor-doped band-gap material can enhance the overall HHG efficiency by several orders of magnitude, compared with undoped and acceptor-doped materials. This enhancement originates from the highest-occupied impurity state which has an isolated energy located within the band gap. The donor-type doping results in a harmonic cutoff different from that in the undoped and acceptor-doped cases, explained by semiclassical analysis for the impurity-state HHG. In the case of an imperfect crystal, we find that disordered systems emit suppressed harmonics in the first plateau region and enhanced harmonics in the second plateau region. The suppression of harmonics in the first plateau becomes less pronounced when introducing a lower level of disorder, while the enhancement in the second plateau region seems insensitive to the level of disorder. The universality of our findings is demonstrated for many disordered sample systems and for different laser field strengths. In addition, a time-frequency profile of HHG spectra shows that the emission of harmonics is less regular in time domain for a disordered system.

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