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Tailoring High-Order Harmonics: A Computational Approach Based on Time-Dependent Density-Functional Theory ALBERTO CASTRO, Department of Physics, Free University of Berlin, ALI AKBARI, ANGEL RUBIO, Universidad del Pais Vasco, EBERHARD GROSS, Department of Physiks, Free University of Berlin — Atoms and molecules react in complex manners when they are irradiated with high-intensity electromagnetic pulses: multi-photon, tunnelling and over-the-barrier ionisation, laser driven photo-induced isomerisations or fragmentations, and high harmonic generation are some of the non-linear effects that are observed. The so-called pulse shaping techniques can be used to design pulses that produce a desired effect. A technologically appealing possibility is to tailor the harmonic emission spectrum: enhancement of some given orders, supressions of others, etc. We have undertaken the task of exploring this possibility from a theoretical point of view, by making use of time-dependent density-functional theory to describe the electrons, a real-space numerical representation, and various optimization techniques.

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