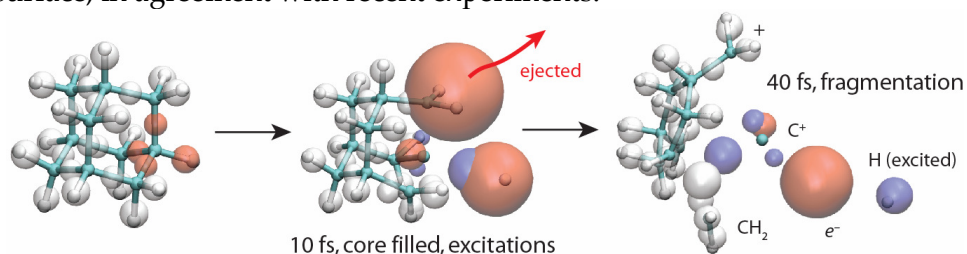


## Simulation of large-scale excited electron dynamics

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To study electron dynamics in large-scale highly excited systems, we have developed eFF, a molecular dynamics model which includes electrons. In eFF, electrons are represented by Gaussian wave packets whose size and position vary with time, and the nuclei are represented by point charges. The particles interact via an effective potential which is so simple that forces acting between thousands of nuclei and electrons can be computed in less than a second on a modern processor. Using eFF, we explore the thermodynamics of warm dense hydrogen [1], and find excellent agreement with path integral methods and diamond anvil and shock compression experiments over a temperature range of 0 to 100,000 K and densities up to 1 g/cm<sup>3</sup>. Hugoniot curves for shock-compressed lithium and beryllium are in good agreement with experiment as well. We also simulate the Auger process (Figure 1) in a diamond nanoparticle (C<sub>196</sub>H<sub>112</sub>), and discover direct and indirect pathways for the desorption of atomic fragments from the surface, in agreement with recent experiments.



**Figure 1.** Auger process in adamantane. After a core electron is ionized from a tertiary carbon at time zero, a valence electron fills the core, another valence electron is ejected, and the molecule fragments over tens of fs.

[1] J. T. Su and W. A. Goddard III, *Phys. Rev. Lett.* **2007**, 99, 185003.