Roles of Core-Shell and δ-ray kinetics in α-Voltaic Efficiency

Theoretical treatments/computations are essential tools for understanding ionization events and the subsequent relaxation mechanisms. A variety of theoretical treatments are employed here for this purpose, including the *ab initio* Fermi golden rule for the core-shell Auger relaxation rates and the TPP-2M [] model for electron-impact ionization kinetics. We demonstrate that for c-BN, ionization cascades are the dominant relaxation pathway, while core shell Auger relaxation contributes a small but relevant number of secondary electron-hole pairs (and efficiency) for every core-shell ionization event. Moreover, a device is suggested which allows for the topping of the α-voltaic with a thermoelectric generator and its maximum efficiency is found to exceed 25%.

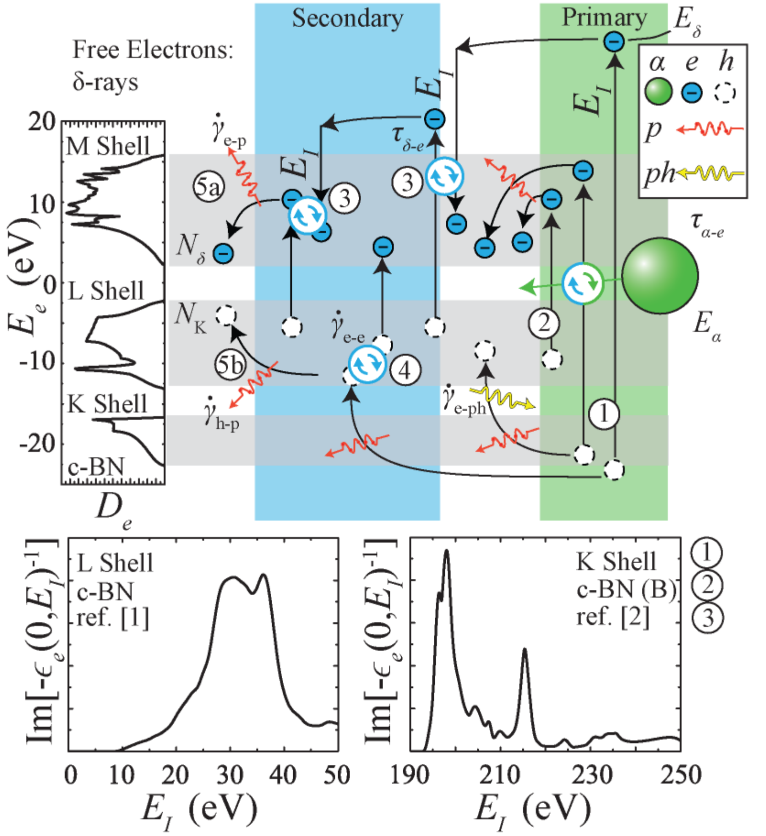

Figure 1. Primary ionization events [core (1) and valence (2)], and their relaxation mechanisms [Impact ionization (3), core-shell Auger relaxation (4), and phonon emission (5)]. Details of the electronic density of states and energy loss functions are also shown.

Impact Ionization

The TPP-2M allows for prediction of the impact ionization kinetics above 10 eV. This is approximately the ionization threshold in c-BN. Thus, we can calculate the mean energy transfer for an impacting δ-ray. This mean ionization energy is used in a semi-analytical scheme to find the number of electron-hole pairs generated for a given primary ionization. This method shows that the average ionization generates pairs with nearly 40% efficiency.

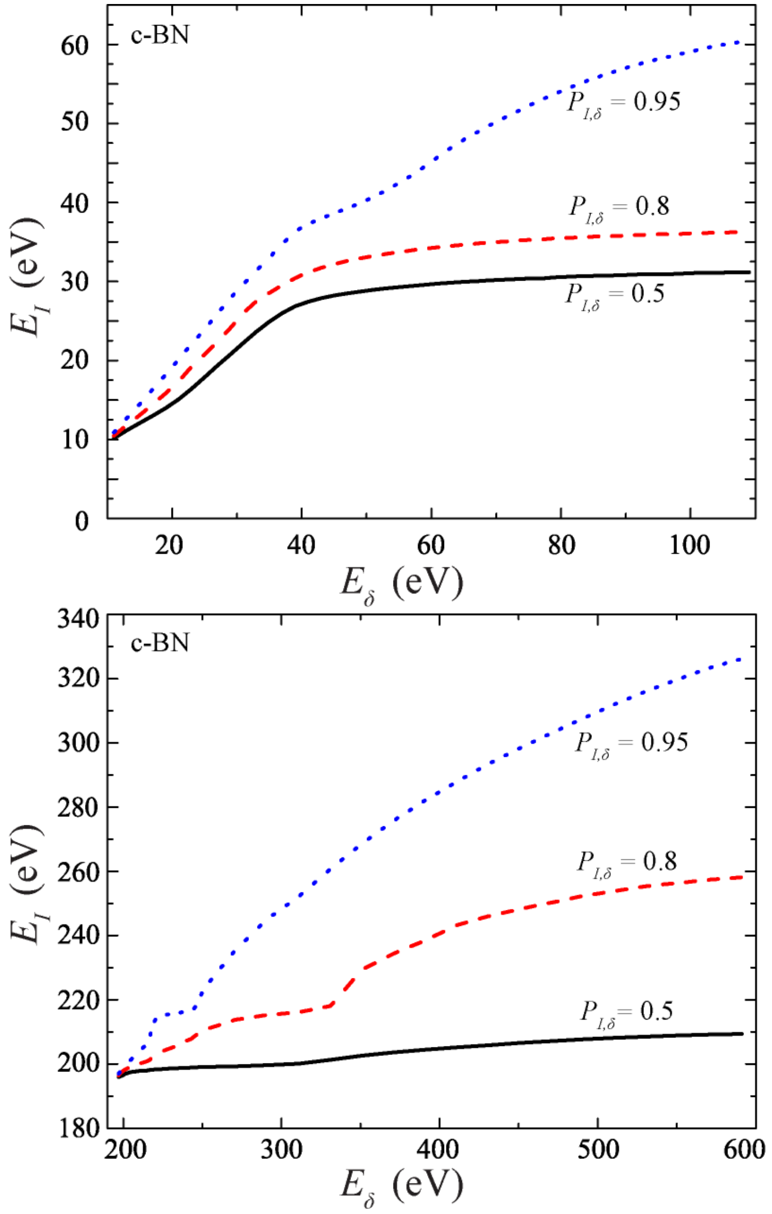

Figure 2. Variations in the probability that a δ-ray of energy E_δ causes an ionization with energy less than or equal to E_I for L (top) and K (bottom) shells. Probabilities of 0.5, 0.8, and 0.95 are shown..

Integrated α-Voltaic -- Thermoelectric

α-voltaic harvest electron-hole pairs generated as energetic α-particles collide with and ionize electrons in a semiconductor. As this is not a thermal cycle, we can top the device with a thermoelectric generator (TEG). However, in order to mitigate radiation damage while creating a significant heat flux for the TEG, a 100 to 1000 times concentration in heat is required. We propose the device shown in Fig. 3, where layers of larger α-voltaic are stacked and a sheath of copper carries the heat to a small TEG and electricity out of the device.

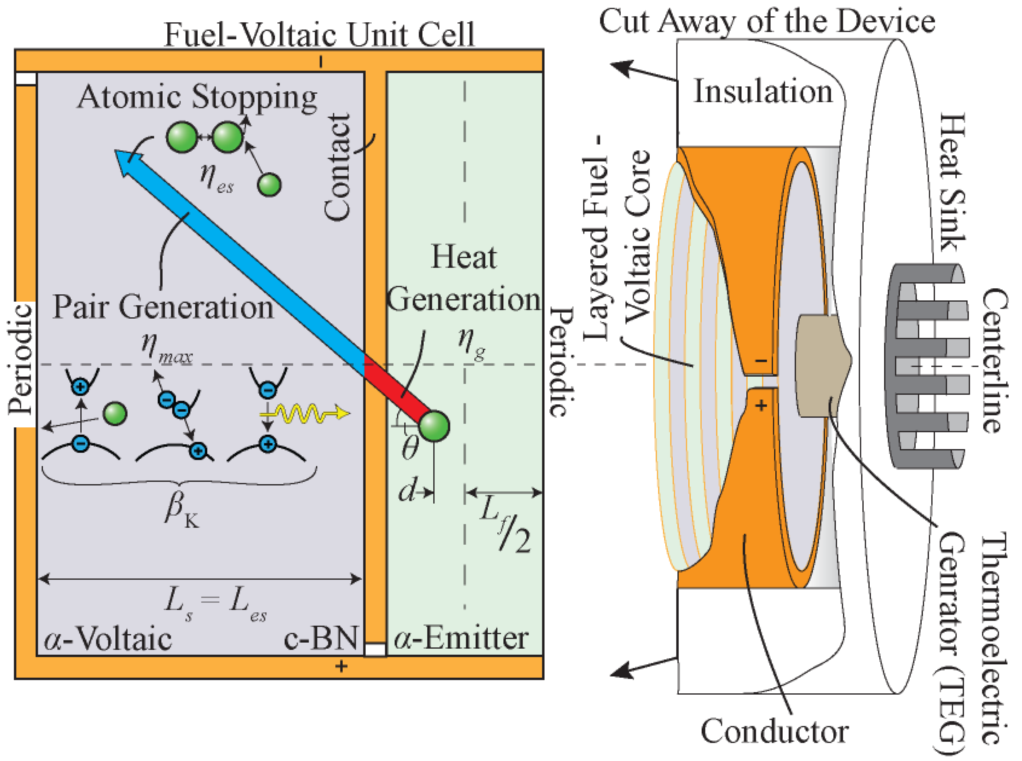

Figure 3. An integrated α-voltaic -- thermoelectric device design . The device concentrates the heat generated in the device and funnels it through the TEG in order to meet its thermal requirements and maintain a reasonably efficient life-span

Core-Shell Kinetics

The core-shell kinetics (Auger and radiative) in c-BN are evaluated using the *ab initio* code VASP and the Fermi golden rule for a variety of carrier concentrations and temperatures. We find that Auger relaxation is favored at higher temperatures and lower concentrations. When combined with the impact ionization results, we find that the core-shell Auger relaxation can add approximately 1% efficiency to primary ionization events.

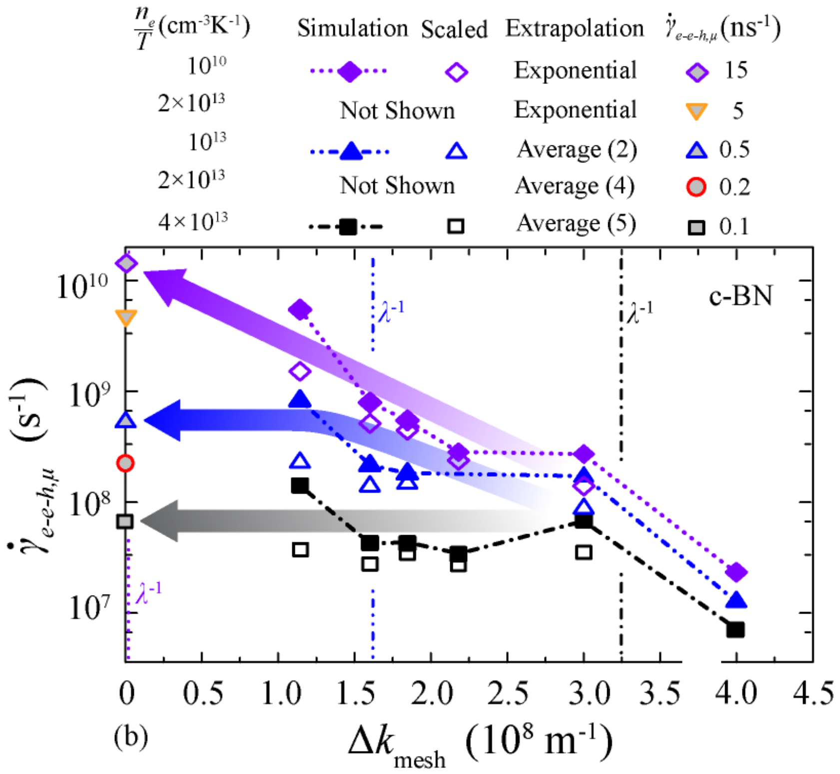

Figure 4. Variations in the average Auger and scaled Auger relaxation rates as a function of the simulation discretization (k-mesh density).