Optical Absorption of Carbon-Metal Nanocomposites

G. Hadjisavvas[1], G. Tritsaris[2], C. Mathioudakis[1], E. Kaxiras[2], and P. C. Kelires[2*]
[1]*Research Unit for Nanostructured Materials Systems, Department of Mechanical and Materials Science Engineering, Cyprus University of Technology, P.O. Box 50329, 3603 Lemesos, Cyprus,*
[2] *Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

Carbon-based materials, including diamond-like carbon (DLC), have been suggested as promising materials for solar energy harvesting. The properties of DLC may be tuned by the incorporation of transition metal atoms, either dispersed or forming nanoparticles. In a recent work [1], we studied DLC/metal nanocomposites, with metal atoms (Ag, Cu) dispersed in the matrix at substitutional sites. We used 64-atom computational cells and density functional theory (DFT) calculations. We found that metal inclusions enhance the optical absorption in the visible, but lower the sp3 fraction and thus the strength and hardness of the DLC matrix. Here, we extend these studies to the nanoparticle case. We start with metal atoms inserted in the DLC matrix interstitially, which eventually grow into larger nanocrystals. We use larger cells of 512 atoms. The initial DLC networks are generated with tight-binding calculations. The final structures with metals are relaxed with DFT and then properties are calculated. The first results indicate that the reduction of sp3 fraction is less drastic than in the dispersed case, which is beneficial for the mechanical properties. Also, the optical absorption is enhanced. By decomposing the absorption coefficient into site contributions, we aim to identify the strong absorbing atoms in the system, especially in the metal nanocrystals.

References

[1] G. Tritsaris, C. Mathioudakis, P. C. Kelires, and E. Kaxiras, J. Appl. Phys. 112, 103503 (2012).

* pantelis.kelires@cut.ac.cy