Diamond-like carbon-metal nanocomposites for solar thermal energy

GEORGIOS TRITSARIS, EFTHIMIOS KAXIRAS, Harvard University, KAXIRAS RESEARCH GROUP TEAM — Solar thermal energy systems are a possible technology for clean energy production. Carbon-based materials, including diamond-like carbon (DLC), have been suggested as promising for solar energy harvesting [1]. A strategy for tuning the properties of DLC is the incorporation of transition metal nanoparticles in the material [2]. Using density functional theory calculations, we study the structural, mechanical, and optical properties of DLC with transition metal nanoinclusions such as silver and copper. Key properties of the nanocomposites, such as the sp$^2$/sp$^3$ bonding ratio, elastic properties, and optical band gaps are reported. Such carbon-metal alloys are calculated to show enhanced performance over DLC.