## Physico-chemical nanomaterials science

# A Computational Study on the Some Physical Properties of B, N and Al Doped Coronene Molecule

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The Coronene (superbenzene or hexabenzobenzene) molecule is a polycyclic aromatic hydrocarbon consisting of flat ring of six fused benzene rings with chemical formula $C_{24}H_{12}$. It can be used as organic light emitting diode (OLED) and low cost graphene synthesis [1,2].

We modified central benzene ring of coronene molecule by introducing B, N, or Al atoms or borazine ring. We have studied the structure, energetic, electronic and optical properties of coronene and its various derivatives including B, N, Al, and borazine substitution. All calculations were performed using density functional theory at the B3LYP/6-31g(d,p) level. B and Al have changed structure substantially, borazine has little effect relatively.

1. *Mathews M., Achalkumar A.S., Li Q.* Self assembled 1D semiconductors: Liquid crystalline columnar phase // Anisotropic Nanomaterials -2015.-P. 241-287.
2. *Wu T., et al.* Continuous graphene films synthesized at low temperatures by introducing coronene as nucleation seeds// Adv Nanoscale-2013.-**5.**-P. 5456-5461.