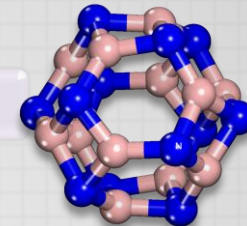




# Ab initio study of the binding of aryl and alkyl radicals onto the $B_{12}N_{12}$ nanocage cluster and g- $C_3N_4$ monolayer

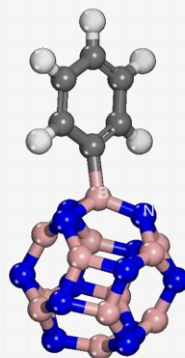
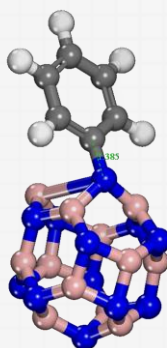
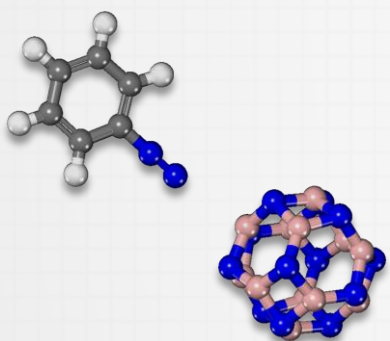


*Asoc. Prof. Avni Berisha - Department of Chemistry, University Of Prishtina, Kosovo*

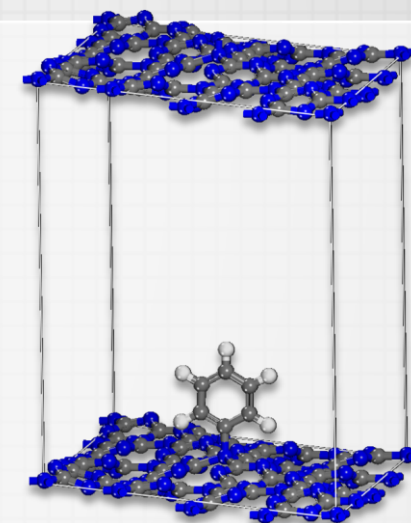
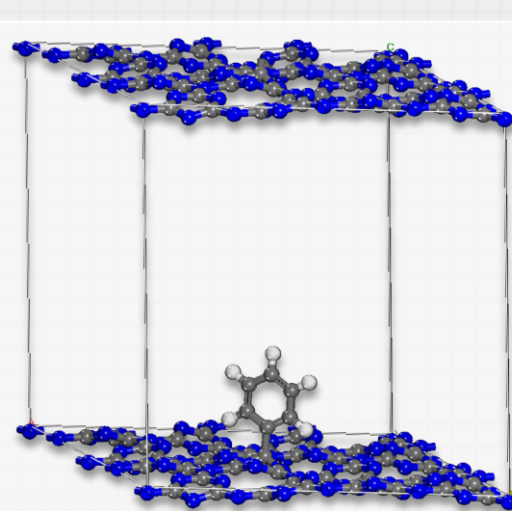
## Introduction

**Boron nitride (BN)** is a refractory material of great importance with valuable thermal and chemical properties. It finds widespread use such as lubricant (at low and elevated temperatures), semiconductor devices, sensing material, etc. **2D graphitic carbon nitride (g- $C_3N_4$ )** among other uses it is an important material as water splitting photocatalyst. For many of these diverse applications, a crucial step for the use of these materials is their surface modification. This is reasonably easily accomplished by the covalent bonding of radicals derived from diazonium salts. Despite experimental evidence, the grafting of alkyl and aryl groups onto the boron nitride surface and g- $C_3N_4$  remains to be addressed concerning their geometry, binding strength, nature of the formed bond, and the activation energy for such a process to take place. To elucidate the grafting process and to better evaluate the formed grafted interface we used Periodic and non-periodic DFT calculations. As a study model for this purpose served monolayer of g- $C_3N_4$  (based on triazine) and a  $B_{12}N_{12}$  nanocage cluster (grafted on both N and C atoms).

## Results



Adsorption of phenyldiazonium || Grafting of phenyl radicals onto  $B_{12}N_{12}$  clusters: N vs. C atoms



Adsorption of phenyldiazonium || Grafting of phenyl radicals onto g- $C_3N_4$  monolayer: N vs. C atoms

## Conclusion

The first step prior to their grafting is the adsorption of the alkyl- or aryldiazonium salts. The formed aryl and alkyl radicals strongly interact with the interface giving bonded alkyl or aryl moieties. The relatively high values of calculated Bond Dissociation Energies (BDE) indicate that during this grafting reaction these radical are covalently attached to the  $B_{12}N_{12}$  nanocage clusters and the g- $C_3N_4$  monolayer.