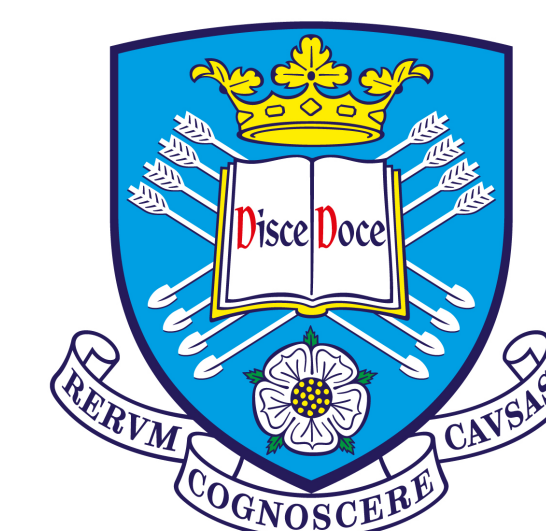


# Calculations on the adsorption of C, O, and N atoms on Graphene

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## Background

- The interstellar medium is a chemically-rich region of the universe.
- Dust particles (consisting of graphitic, silicate material) allow for heterogeneous catalysis in the ISM.
- Adsorption of (H, C, O, and N) atoms is the first step in such a process.
- From the literature (adsorption of H), coronene is used as a model for graphene. This comparison has not been made for other atoms.
- Few studies have been done on the importance of dispersion forces.



Figure 1: Interstellar clouds in central region of Milky Way galaxy : Spitzer Telescope

## Computational methods

Coronene

- Scan, optimization: Gaussian09, E01.
- B3LYP/6-311G(d, p)
- B3LYP-GD3(BJ)/6-311G(d, p).
- DFT

Graphene

- Optimization-VASP v.5.4.4.
- PAW-PBE/Plane wave.
- DFT

## References

- M. Saez and F. Ruette, CPL, (2015), 640, 11-15.
- L. Jelaica, V. Sidis, CPL, (1999), 300, 157-162.
- F. Dulieu and et al., A&A, (2010), 512, A30.

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## Results

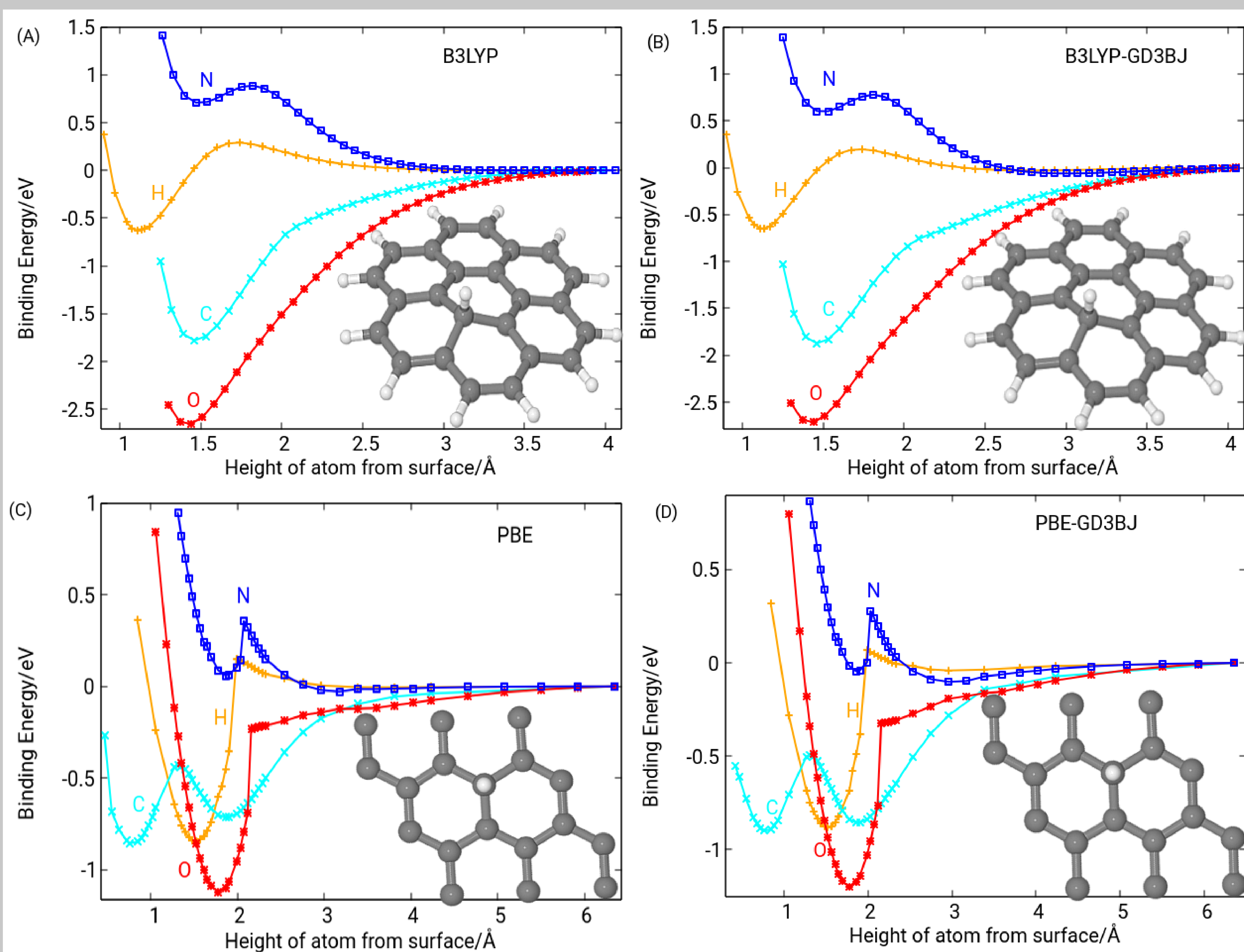


Figure 2: Binding energy of H, C, N, and O atom as a function of distance

- Panel (A)- Coronene
- Panel (B)- Coronene with empirical dispersion
- Panel (C)- Graphene
- Panel (D)- Graphene with empirical dispersion

## Conclusions

- Hydrogen shows non-activated physisorption only with dispersion correction which is also mentioned in many previous research.
- Interactions of C and O with coronene surface shows chemisorptions without energy barrier, whereas N does not show any interaction with coronene.
- H and O adsorption behavior is similar on graphene surface as with coronene.
- Interaction of C on graphene shows double well, while N shows physisorption.
- Adding dispersion correction improve adsorption energy results with all.

## Future work

- Study of interactions of C, O, N and other atoms and molecular gases on Bi-layer graphene surface.
- Study of reactions of atoms on pre-adsorbed surface.
- Comparisons of results of graphene and PAH interactions.



Figure 3: Carina nebula, pillar with glow of O(blue), H & N(green), and S(red): ESA/Hubble Telescope



Figure 4: Dark molecular cloud, Barnard 68: FORS, VLT/ ESO