Universitat Autònoma de Barcelona

QUANTUMGRAIN
Quantum Chemistry on Interstellar Grains

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Binding Energies of Interstellar Complex Organic Molecules on Crystalline Water Ice Surface

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INTRODUCTION

Objective: A robust yet cheap hybrid methodology to obtain accurate energies for large systems

MOLECULAR CLOUDS

- Cold and dense star-forming regions or "stellar nurseries"
- Composed of gaseous molecules and submicron dust grains
- Carbonaceous or silicate dust grains are covered with water-dominant ice mantles

Figure 1. "Cosmic Cliffs", the edge of a young star-forming region in the Carina Nebula. Image taken by JWST (Credits: NASA, ESA, CSA, and STScI)

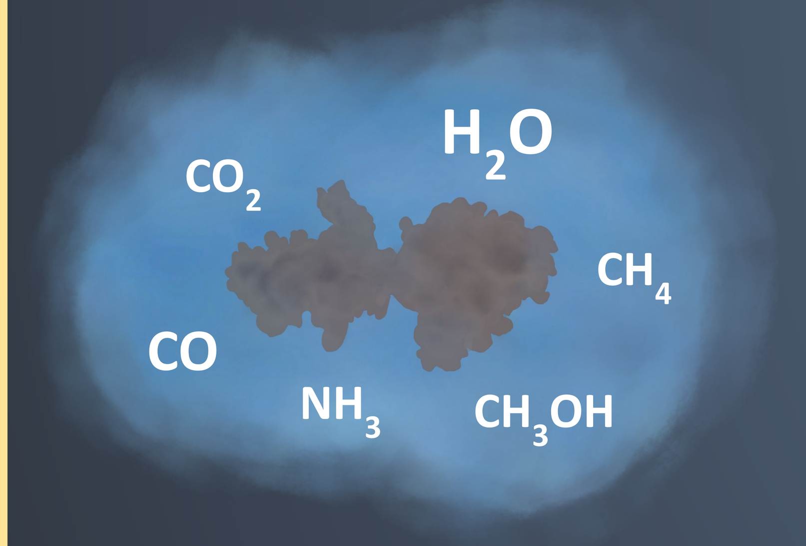


Figure 2. The structure of an interstellar dust grain (Credits: Hunarpreet Kaur)

GRAIN SURFACE CHEMISTRY

- Molecules accrete, diffuse, and react on the icy mantles
- Astrochemical models require accurate binding energies as input parameters

INTERSTELLAR COMPLEX ORGANIC MOLECULES (iCOMs)

- Molecules containing more than 6 atoms and at least one C
- Out of approximately 270 observed interstellar molecules, nearly 40% are iCOMs
- Potential link between interstellar chemistry and the emergence of life on Earth

METHODS

METHODS FOR BE CALCULATION

Density Functional Theory: **B3LYP-D3(BJ)/Ahlrichs-TVZ**

Refinement using **CCSD(T)** with an ONIOM2-like approximation

Cost-effective methodology: **DFT//HF-3c**

HF-3c optimization followed by single-point energy calculation using DFT

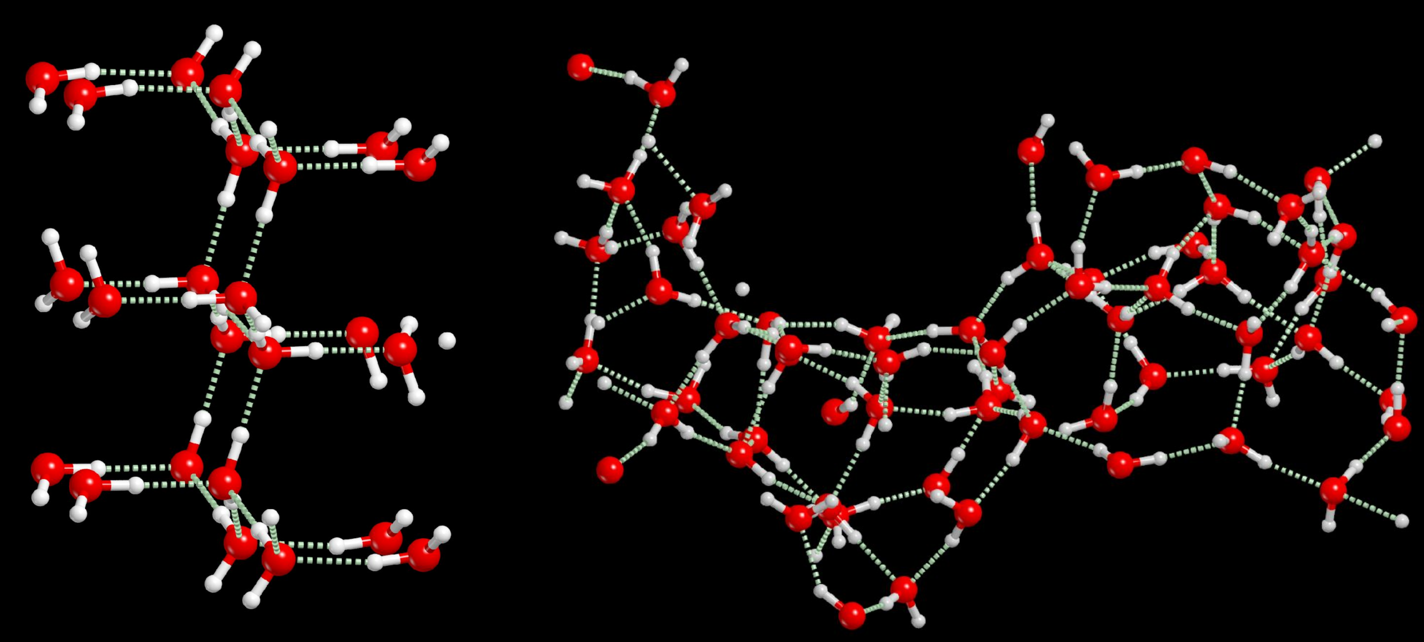
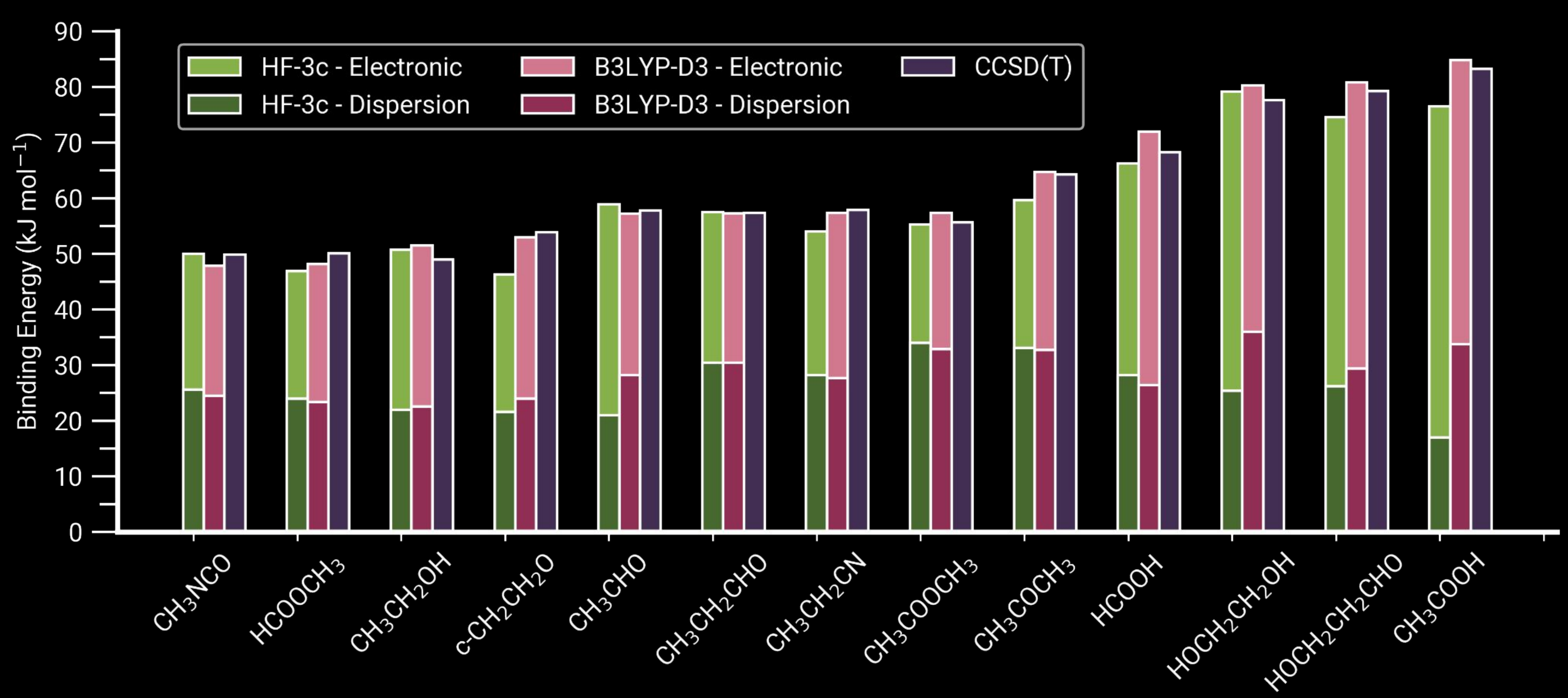


Figure 3. Proton-ordered crystalline (010) water ice and amorphous water ice



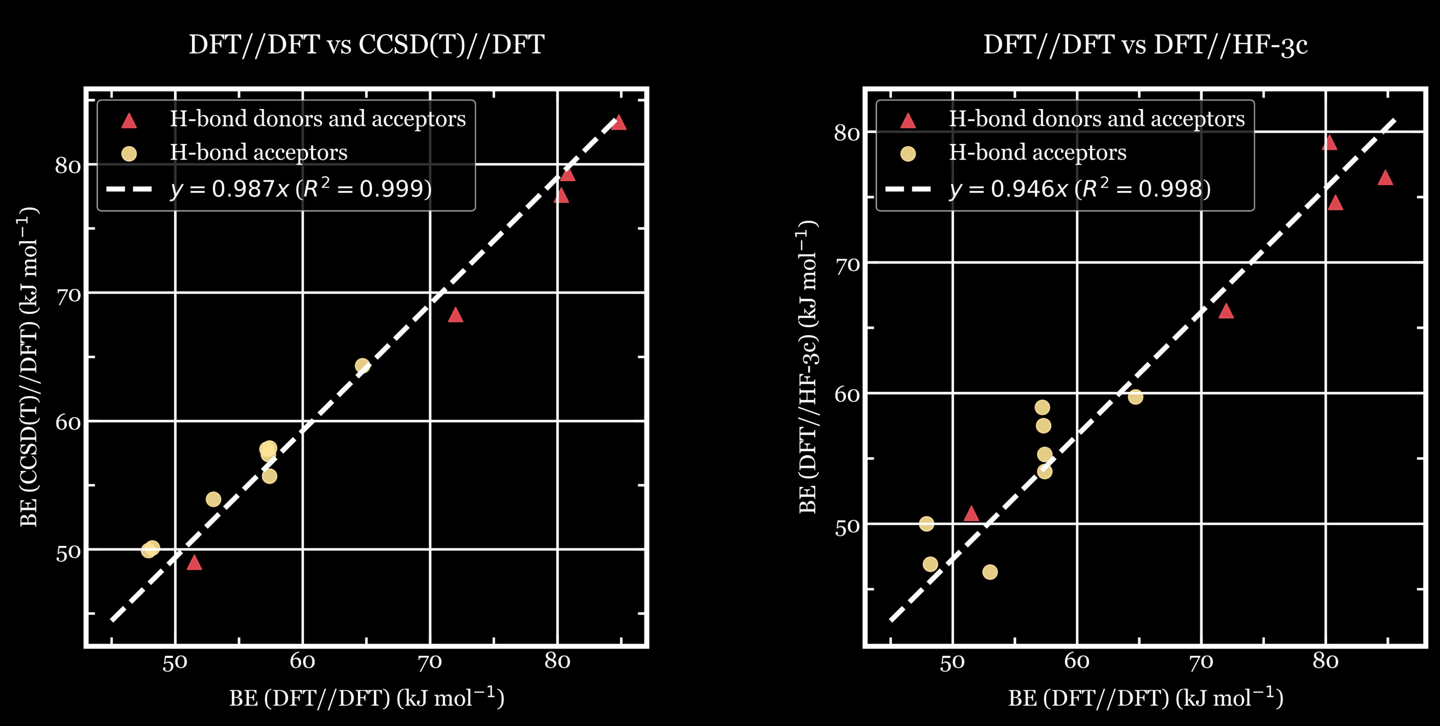


Figure 4. Correlation among the BEs obtained using B3LYP-D3 (DFT), CCSD(T), and the hybrid DFT//HF-3c methods

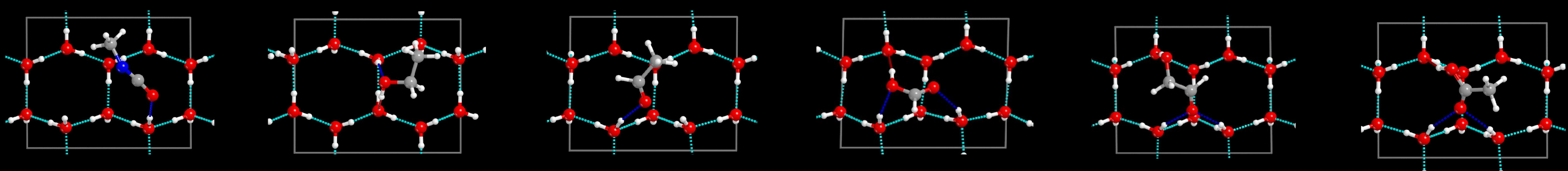


Figure 5. Adsorption of CH_3NCO, CH_3CH_2OH, CH_3CHO, HCOOH, $HOCH_2CHO$, and CH_3COOH on crystalline water ice surface

CONCLUSIONS

Strong H-bond cooperativity (non-dispersive interactions) leads to higher BE values

Dispersion contribution is lower in iCOMs with higher BEs

PERSPECTIVES

The ices in the ISM are predominantly present in the amorphous state. To account for variable binding sites and the lack of long-range order, we require a larger unit cell.

The hybrid DFT//HF-3c methodology allows for cost-effective calculations without compromising on the accuracy.

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