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Szanowni Państwo,

w dniach 12.06-16.06.2023 naszym gościem na Wydziale Chemii UWr będzie Pani Profesor Célia Fonseca Guerra (VU Amsterdam). W dniach 13.06-15.06 Pani Profesor wygłosi serię wykładów, a także odbędą się warsztaty z pracy z programem ADF. Na następnej stronie przedstawiamy ogólne streszczenie cyklu wykładów wraz z dodatkową szczegółową literaturą przedmiotu.

Bardzo prosimy, aby osoby zainteresowane warsztatami skontaktowały się z dr hab. Anetą Jezierską, prof. UWr, gdyż liczba miejsc jest ograniczona i będzie decydowała kolejność zgłoszeń (warsztaty są planowane w sali komputerowej 17a).

Wykłady będą się odbywać w sali I BB:

13.06.2023 - wtorek – 16:00-19:00 – Lecture 1 and 2
14.06.2023 - środa – 16:00-19:00 – Lecture 3, 4 and 5
15.06.2023 - czwartek – 15.30-16.30 – Lecture 6 oraz 17:00-19:00 – warsztaty w sali 17a.

z wyrazami szacunku,
Aneta Jezierska & Jarosław J. Panek

Ladies and Gentlemen,

between June 12th and June 16th Professor Célia Fonseca Guerra (VU Amsterdam) will be the guest of our Faculty of Chemistry. In the period 13.06-15.06 Professor Fonseca Guerra will present a series of lectures, and a workshop session will be held devoted to the ADF program. The following page contains a general abstract of the lecture series together with additional literature references for further reading.

The persons interested in the workshop are kindly asked to contact DSc. Aneta Jezierska, Prof. UWr, because the attendance is limited by the number of places in the computer room and the registration will be based on the “first come first registered” basis (the workshop is planned to be held in the computer lab 17a).

The lectures will be held in the Lecture Hall I BB:

13.06.2023 - Tuesday – 16:00-19:00 – Lecture 1 and 2
14.06.2023 - Wednesday – 16:00-19:00 – Lecture 3, 4 and 5
15.06.2023 - Thursday – 15.30-16.30 – Lecture 6, and 17:00-19:00 – the workshop in the lab 17a.

with kind regards,
Aneta Jezierska & Jarosław J. Panek

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Lecture series

1. Understanding Hydrogen bonds in DNA with KS Molecular Orbital Theory

2. Guanine Quadruplexes: Role of Cooperativity and Cations

3. Cooperativity proves Covalency in Hydrogen Bonds and Halogen Bonds

4. Importance of Pauli Repulsion and Secondary Electrostatic Interactions in Hydrogen Bonds

5. How Chalcogen Atom Size determines hydrogen bonding and polymer formation.

6. Lewis Acid/Base Interaction and Metallophilicity

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Hydrogen bonds are omnipresent in biological and supramolecular chemistry. Nevertheless, they are still mostly represented in an oversimplified manner (positively charged hydrogen attracts close-by negatively charged heteroatom) which is easy to use but often fails to explain or even qualitatively reproduce experimental findings. In my lecture series, I present a state-of-the art physical model, based on quantitative molecular orbital theory, which enables a quantum-mechanically sound, yet intuitive approach to the interesting complexity of the hydrogen bond. The latter can be dissected into understandable contributions such as covalent bonding and Pauli repulsion between occupied orbitals. Complex and seemingly exotic phenomena are unraveled and explained in a unified manner:
- Nature of bonding in DNA[1]
- cooperativity in quadruplex structures of DNA and linear chains of squaramides,[2]
- variations in bond lengths and energies due to steric repulsion,[3]
- the legitimacy of the secondary electrostatic interaction model [4]
- the hydrogen bond donor capability of carboxamides for supra-molecular chemistry.[5]
- other donor-acceptor interactions: boron and nitrogen trihalides and metallophilicity .[6]

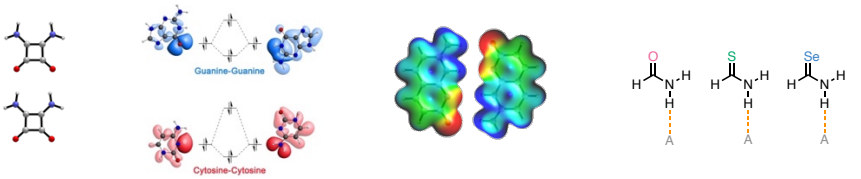

Fig. 1. Different aspects of the nature of hydrogen-bonded systems.

References

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