

2019 International Solvay Chair in Chemistry



Professor Gernot Frenking

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Lecture 3 on Tuesday 5 November (4 - 6 pm, Solvay Room)

CONJUGATION, HYPERCONJUGATION AND AROMATICITY

This lecture focusses on important models for chemical bonding, which are ubiquitously used for the description of molecular structures and reactivities, often without solid fundament but merely used as heuristic pseudo explanation. I will emphasise the difference between a bonding model and the physical mechanism of chemical bond formation. The unobservable concepts of conjugation, hyperconjugation and aromaticity can quantitatively be derived from the terms of an energy decomposition analysis (EDA) which correlate quite well with experimental observations¹ I will also make some critical remarks concerning the frequently made correlation between magnetic current and aromaticity.²

1. (a) I. Fernández and G. Frenking, *Open Org. Chem. J.* 5, 79 (2011); (b) I. Fernández and G. Frenking, *Faraday Discuss.* 135, 403 (2007); (c) I. Fernández and G. Frenking, *Chem. Commun.* 5030 (2006); (d) I. Fernández and G. Frenking, *Chem. Eur. J.* 12, 3617 (2006); (e) D. Cappel, S. Tüllmann, A. Krapp and G. Frenking, *Angew. Chem. Int. Ed. Engl.* 44, 3617 (2005).

2. L. Zhao, R. Grande-Aztatzi, C. Foroutan-Nejad, J. M. Ugalde, G. Frenking, *Chemistry Select* 2, 863 (2017)

Lecture 4 on Tuesday 12 November (4 - 6 pm, Solvay Room)

CHEMICAL BONDS IN DIATOMIC MOLECULES

I will discuss the nature of the chemical bond in some elementary diatomic molecules using charge and energy decomposition methods. Particular attention is paid on the chemical bond in CO and the shortest known bond between any two atomic species heavier than hydrogen and helium.

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