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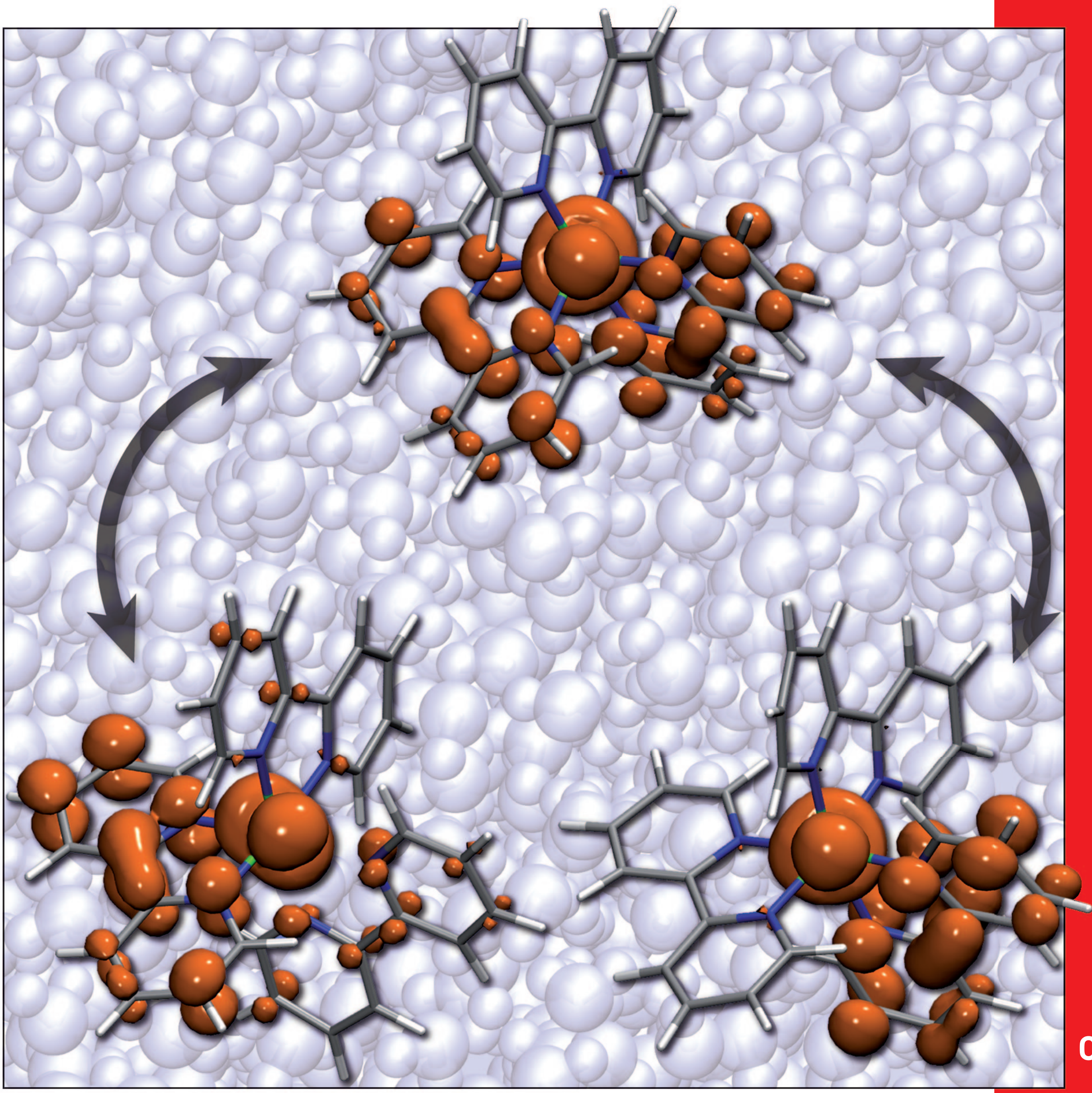

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Concept

Cross-Coupling Cyclization Reactions
of Two Different Allenic Moieties

B. Alcaide, P. Almendros and T. Martínez del Campo

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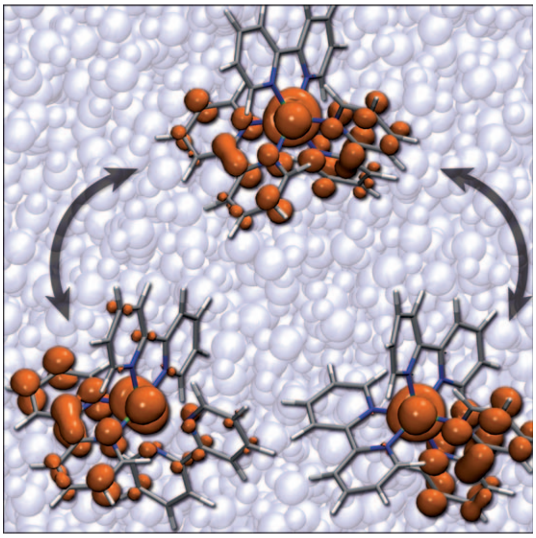
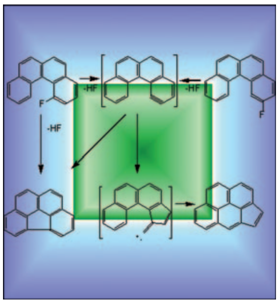
Solvent-induced…

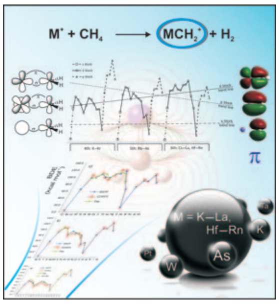
… electron localization and dynamics in the triplet metal-to-ligand charge-transfer (^{3}MLCT) state of $[Ru(bpy)_3]^{2+}$ (bpy = 2,2′-bipyridine) have been investigated by means of Car–Parrinello QM/MM simulations. In the gas phase, the unpaired electron is found to be delocalized over the three bipyridine ligands, but in solution the excited electron is, most of the time, located on a subset of ligands. More details can be found in the Full Paper on page 5889 ff. by I. Tavernelli et al.



Cyclization/Coupling Reactions
In their Concept article on page 5836 ff., B Alcaide, P. Almendros, and T. Martínez del Campo show that cross-coupling/cyclization reactions with two different allene derivatives are a powerful method for the direct synthesis of functionalized butenolides, furanimines, and 2,5-dihydrofuran derivatives. The directness of this allene-based approach, which permits great flexibility in selection of different coupling partners, coupled with the versatility of the reactions, are impressive advantages that should facilitate the synthesis of many useful molecules.

C−C Coupling
In their Communication on page 5868 ff., K. Yu. Amsharov et al. show that HF homo-elimination can be an efficient approach for intramolecular aryl–aryl coupling, for example, in closing five-membered rings in polycyclic aromatic hydrocarbons. The through-space fluorine activation mechanism has been identified experimentally and confirmed by quantum chemical calculations.





Periodic Trends
In their Full Paper on page 5882 ff., X. Zhang and H. Schwarz describe the DFT analysis of 54 cationic methylene complexes MCH_2^+ (M = K–La, Hf–Rn), which reveals different bonding trends for s-, p-, and d-block elements.

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