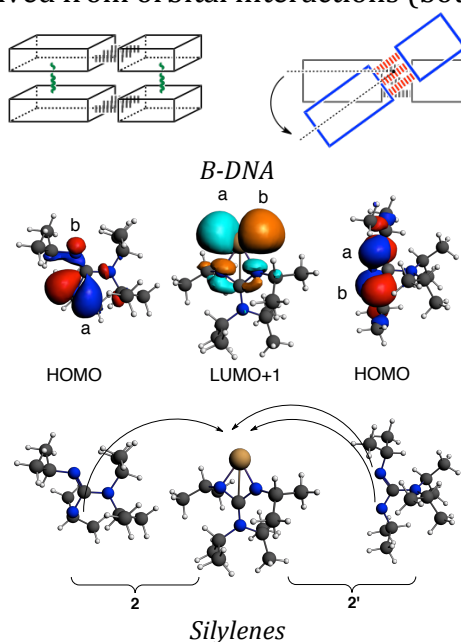


B-DNA Structure and Stability & Silylenes Stability and Reactivity through DFT Bonding Analyses

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Structural and bonding analyses based on quantitative molecular orbital DFT have been applied to study the structure and stability of B-DNA, and the stability and reactivity of silylenes. First, the bonding in a series of 47 stacks consisting of two base pairs, in which the base pairs cover the full range of natural Watson-Crick pairs, mismatched pairs, and artificial DNA base pairs have been analyzed. The analyses provide detailed insight into the role and relative importance of the various types of interactions, such as, hydrogen bonding, π - π stacking interactions, and solvation/desolvation (top figure).^[1] On the other hand, donor-stabilized bis(amidinato)silicon(II) **1** and bis(guanidinato)silicon(II) **2** have been recently synthesized, showing different chemical reactivity. Both silylenes are three-coordinate in the solid state, whereas **1** is four-coordinate, and **2** three-coordinate in solution, also confirmed by relativistic DFT computations. The preference for three-coordination of **2** in solution originates from a subtle interplay of factors derived from orbital interactions (bottom figure).^[2,3]



- [1] J. Poater, M. Swart, F. M. Bickelhaupt, C. Fonseca Guerra, *Org. Biomol. Chem.* **2014**, *12*, 4691-4700.
[2] F. M. Mück, D. Kloß, J. A. Baus, C. Burschka, R. Bertermann, J. Poater, C. Fonseca Guerra, F. M. Bickelhaupt, R. Tacke, *Chem. Eur. J.* **2015**, *21*, 1411-1421.
[3] F. M. Mück, J. A. Baus, M. Nutz, C. Burschka, J. Poater, F. M. Bickelhaupt, R. Tacke, *Chem. Eur. J.* **2015**, *21*, 16665-16672.