## KN03

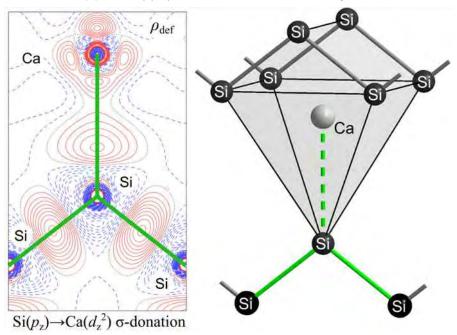
## Charge Density and Chemical Bonding in Inorganic Materials

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Since the theoretical prediction and experimental verification of Charge Concentrations (CCs) in the valence shell of main group elements and transition metals several attempts have been undertaken to understand their origin and relevance in chemistry and physics. In pioneering studies we could demonstrate that these CCs not only influence the geometry of coordination compounds and solids but also serve as controlling parameters for important chemical reactions like the activation of chemical bonds in catalytic reactions [1]. Furthermore, in covalent solids such as transition metal oxides and carbides they appear to signal even subtle electron localization phenomena which might induce metal-to-insulator transitions or effect the onset of superconductivity [2]. The complex interplay between valence shell charge concentrations and chemical properties of molecules and solids will be the central topic of this contribution with the focus on (i) unusual bonding scenarios displayed by solid state compounds [3] and the (ii) control of geometry and bond activation processes in molecules.

[1] W. Scherer, P. Meixner, J. E. Barquera-Lozada, et al., Angew. Chem. Int. Ed. 2013, 52, 6092-6096., [2] W. Scherer, Ch. Hauf, M. Presnitz, et al., Angew. Chem. Int. Ed. 2010, 49, 1578–1582., [3] I. M. Kurylyshyn, T. F. Fässler, A. Fischer, et al. Angew. Chem. Int. Ed. 2014, 53, 3029-3032.



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