

## Dash, arrow, dotted line – any evidence for these heuristic principles from charge density?

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Ever since G. N. Lewis invented the dash between two elements to define the two-centre-two-electron bond 99 years ago this concept proves to be most resilient among the various disciplines of chemistry. It is the lowest common denominator and works best in organic chemistry. Even the reactivity of substrates and the variety of products can to a certain extent be explained and predicted by weighting the canonical forms. Anyhow, there is no dash in nature and the chemical bonding is wide open to discussion, prone to implement various codes for interactions like the arrow for donor bonds and the dotted line for weak interactions, e. g. hydrogen bonding. The electron deficient bonds e. g. in boron compounds are particularly difficult to rationalise.

The talk will provide some physically meaningful insights from charge density investigations and discuss the chemical re-translation to reactivity, among them low valent silicon,<sup>[1]</sup> (hetero)aromatic systems<sup>[2]</sup> and reactive organometallics.<sup>[3]</sup>

Some of these cases can be covered by Lewis diagrams, others not. They are a good start to explain bonding, but certainly anticipated, mostly too limited in others.

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[2] J. Hey, D. Leusser, D. Kratzert, H. Fliegl, J. M. Dieterich, R. A. Mata, D. Stalke, *Phys. Chem. Chem. Phys.* **2013**, *15*, 20600–20610.

[3] J. Hey, D. M. Andrada, R. Michel, R. A. Mata, D. Stalke, *Angew. Chem.* **2013**, *125*, 10555 –10559; *Angew. Chem. Int. Ed.* **2013**, *52*, 10365 –10369.

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