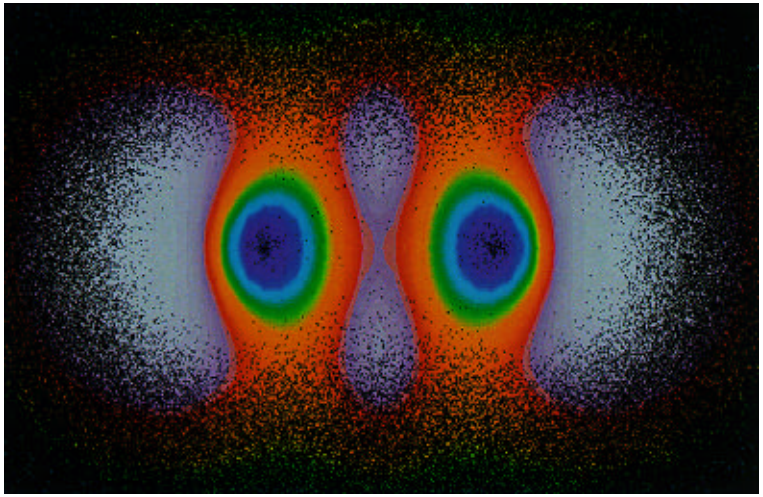
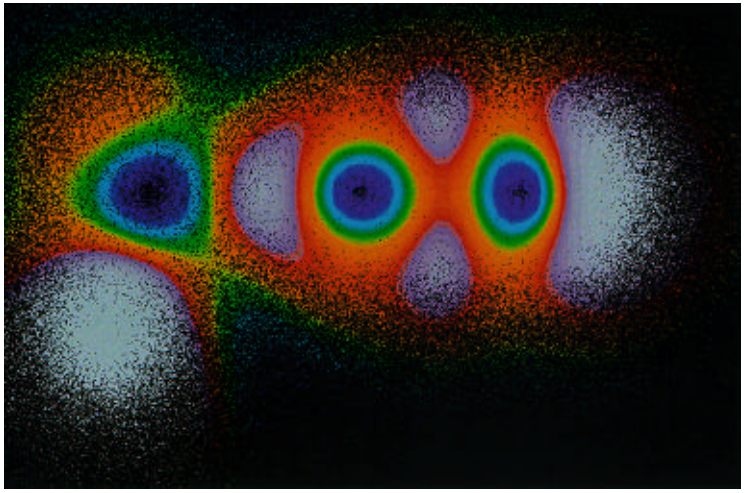
CONCLUSION

Graphical presentations of color-coded gradient vector fields of electron density functions in real 3-dimensional Cartesian space allow for bonding analysis based on the total electron density distribution. With the availability of such graphical tools for the analysis of the total electron density (TED) function — which is an "observable" and which can be measured experimentally — it is hoped that simplistic MO analysis will eventually be replaced by TED analysis. The analysis of the cation-dinitrogen interactions exemplifies well that the CCGVF presentations of the TED functions capture the essence of rather diverse bonding situations without any external reference and without any approximation. Covalent, dative and electrostatic C-N bonding are clearly distinguished by the anisotropies (described by the GVF line shape and density) and by the symmetry and magnitude of the density (color coding) in the bonding regions. The replacement of MO by TED analysis does not mean that valued concepts will be lost. Concepts that are firmly based on quantum-mechanical principles persist in TED analysis in a more rigorous form. For example, as chemists we are fundamentally concerned with electron pairs and these can be recovered in TED analysis via the electron localization function. In collaboration with Dr. Faessler, we are currently studying C-N bonding with electron localization functions which bring to the fore the engagement of the lone pair of N_2 in bonding.

Electron Localization Functions (ELF)
Comparison of Dinitrogen and Methyldiazonium Ion





N≡N	[Me—N≡N]$^{+}$

White areas in the ELF functions indicate bonding electron pairs or lone pairs. Note the extended white areas found for dinitrogen in the regions of the lone pairs. In particular, these plots clearly bring to the fore the fact the dative nature of the C-N bond in methyldiazonium ion. There clearly is a kidney-shaped white area in the C-N bonding region of the ELF function of methyldiazonium ion.

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