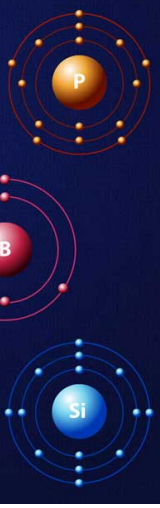
Prem C
Conferences, Events & Workshops

PBSi 2017

International Conference On
Phosphorus, Boron and Silicon

July 3-5, 2017 | Paris




# Impact of boron and phosphorus on the optical properties of organic compounds. A theoretical approach

PROF. JEAN-FRANCOIS HALET
Institut des Sciences Chimiques de Rennes, UMR 6226 CNRS-Ecole Nationale Supérieure de Chimie de Rennes-Université de Renne

Many π-conjugated systems containing hetero-elements such as acceptor three-coordinate boron[1] or hypervalent phosphorus[2] for instance, display strong linear and/or non-linear optical properties, making them suitable for many potential applications. Interestingly, the electronic properties of these compounds can be easily tuned by varying the surrounding substituents tethered to the hetero-elements. Density-functional theory (DFT) calculations of the ground and excited states of a selection of such boron- or phosphorus-containing systems were carried out to analyze and interpret some of their properties.[3] Case studies will be shown and discussed.

REFERENCES

[1] See for example Ji, L.; Griesbeck, S.; Marder, T. B. Chem. Sci. 2017, 8, 846 and references therein.
[2] See for example Duffy, M. P.; Delaunay, W.; Bouit, P.-A.; M. Hissler, M. Chem. Soc. Rev. 2016, 45, 5296 and references therein. [3] (a) Yuan, Z.; Collings, J. C.; Taylor, N. J.; Marder, T. B.; Jardin, C.; Halet, J.-F. J. Solid State Chem. 2000, 154, 5; (b) A. K.; Kaiser, H. M.; Kaufmann, D. E.; Poon, S.-K.; Wong, W.-Y.; Jardin, C.; Fathallah, S.; Boucekkine, A.; Halet, J.-F.; Marder, T. B. Chem. Eur. J., 2006, 12, 2758; (c) Entwistle, C. D.; Collings, J. C.; Steffen, A.; Pålsson, L.-O.; Beeby, A.; Albesa-Jové, D.; Burke, J. M.; Batsanov, A. S.; Howard, J. A. K.; Mosely, J. A.; Poon, S.-Y.; Wong, W.-Y.; Ibersiene, F.; Fathallah, S.; Boucekkine, A.; Halet, J.-F.; Marder, T. B. J. Mater. Chem. 2009, 19, 7532; (d) Ji, L.; Edkins, R. M.; Sewell, L. J.; Beeby, A.; Batsanov, A. S.; Fucke, F.; Drafz, M.; Howard, J. A. K.; Moutounet, O.; Ibersiene, F.; Boucekkine, A.; Furet, E.; Liu, Z.; Halet, J.-F.; Katan, C.; T. B. Marder, T. B. Chem. Eur. J. 2014, 20, 13618.