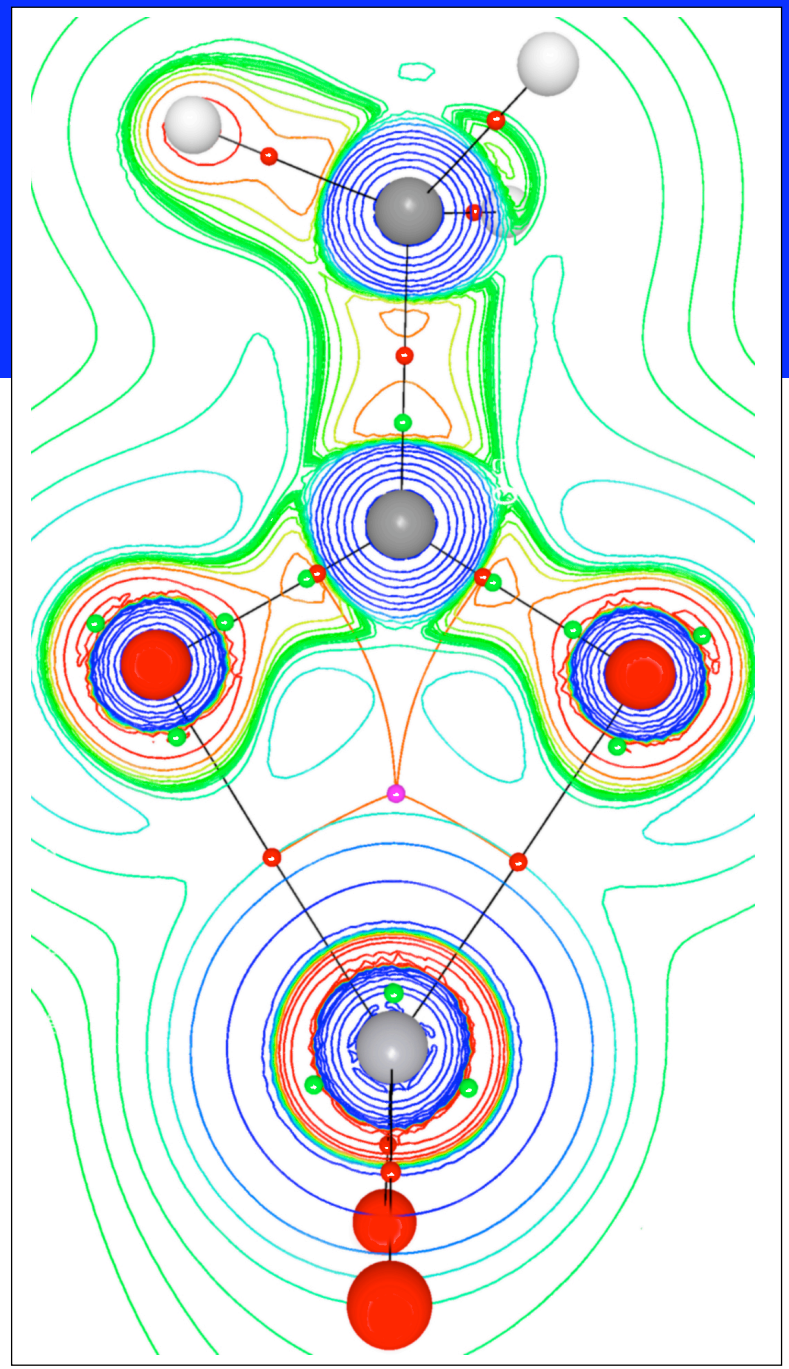
Shedding some light:

How Theoretical Chemists Look at Colourants



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Sala de reuniões do DCR

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Filipe Teixeira is a Theoretical and Computational Chemist with a PhD in Sustainable Chemistry granted by the University of Porto and the Nova University of Lisbon, Portugal, and pre-doctoral experience in Food Chemistry, Organic Synthesis, and Environmental Chemistry. During his graduate research, he approached the difficulties and limitations of the first principles study of Jacobsen catalyst using a combination of Density Functional Theory (DFT), Bader's Quantum Theory of Atoms In Molecules (QTAIM) and Multivariate Analysis techniques. Current research interests include the refinement of Gillespie's VSEPR-derived model for the inner Valence Shell of transition metal atoms and novel theoretical approaches for the study of graphene-derived materials. Vibrational analysis (prediction of Infrared and Raman spectra) and the QTAIM description of inter-molecular interactions, integrate his long-term vision of contributing towards an improved dialogue between different specialities, both in the theoretical and experimental realms.

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