Title	**Learning Chemistry from Electron Densities through Artificial Intelligence**
PI	**Sergio Rampino**
Research Group	**Theoretical Chemistry Group (TCG)**
Curriculum	**Scienze Molecolari**
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Project description:

Chemistry is discussed and rationalized in terms of concepts rooted in quantum mechanics that have their physical counterpart in large, intricate and often opaque data related to the spatial distribution of the electron cloud and produced by solving the equations of either wavefunction or density-functional theory. Venturing in so far unexplored venues for the integration of chemistry, physics and computer science, this PhD project aims at developing a machine-learning framework for the analysis and interpreatation of molecular electron densities obtained by state-of-the-art quantum-chemistry calculations, with a focus on latent relationships between hidden data features and well-established chemical concepts (e.g., atom, bonding, donation, backdonation, hydrogen bonding). Applications will include comparison with conventional bond-analysis techniques and the characterization of molecular systems exhibiting controversial features.

Selected publications:

- Nottoli G, Ballotta B, Rampino S, **Local charge-displacement analysis: targeting local charge-flows in complex intermolecular interactions**, *The Journal of Chemical Physics* 157, 084107 (2022)
- Potenti S, Paoloni L, Nandi S, Fusè M, Barone V, Rampino S, **Chemical bonding in cuprous complexes with simple nitriles: octet rule and resonance concepts versus quantitative charge-redistribution analysis**, *Physical Chemistry Chemical Physics* 22, 20238-20247 (2020)
- Fusè M, Rimoldi I, Facchetti G, Rampino S, Barone V, **Exploiting coordination geometry to selectively predict the σ-donor and π-acceptor abilities of ligands: a back-and-forth journey between electronic properties and spectroscopy**, *Chemical Communications* 54, 2397-2400 (2018)
- Bistoni G, Rampino S, Scafuri N, Ciancaleoni G, Zuccaccia D, Belpassi L, Tarantelli F, **How π back-donation quantitatively controls the CO stretching response in classical and non-classical metal carbonyl complexes**, *Chemical Science* 7, 1174-1184 (2016)

Collaboration network:

Dr Anthony Scemama (Université Paul Sabatier Toulouse III), Prof Stefano Sanvito (Trinity College Dublin), Dr Davide Tiana (University College Cork)