Integrating inferences simulation and deduction in molecular modeling

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Standard molecular modeling is traditionally done via Schroedinger equations via the help of powerful tools helping to manage them atom by atom often needing High Performance Computing

When functional domains are known and for instance Plasmon measured in their specific effects, a simple Galerkin simulation touching all possible configurations for those domains even allows to forecast unknown mutants as in [1] for Sos1, then discovered.

Integrating eXplainable AI in the form of understandable rules Machine Learning [2], one can gain knowledge from data in the predicative logic form

if ... then ... else...,

immediately integrable to the theoretical priors, summing pros of both inference and deduction

[1] E. Sacco, M Farina, C Greco, S Lamperti, S Busti, L DeGioia, L Alberghina, *D.Liberati* and M. Vanoni, *Biotechnology advances* **2012**, *30 (1),* 154-168.
[2] M. Muselli and D.Liberati, *IEEE Trans KDE* **2002**, *14 (6),* 1258-1268.