Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Students' Annual Seminar

Machine Learning models for prediction of X-ray photoelectron spectra of main group molecules

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X-ray photoelectron spectroscopy (XPS) relies on the identification of atomic states via distinct ionisation energies of core-electrons. Owing to the short lifetime of such ionisations, the resolution of such experimental spectra is limited by broadening due to Heisenberg's uncertainty principle. Consequently, the prediction of XPS incorporates the use of ab-initio simulation of XPS for verification. Unfortunately, currently available ab-initio methods for prediction of spectra can be computationally expensive or with numeric instabilities making it challenging to find a perfect method for theoretical prediction. Post a benchmark with tweaks to currently available ab-initio techniques making them robust for accurate automated high-throughput workflow, we have curated an in-house XPS database for the bigQM7w[1] chemical space. This data is used to train atom-specific graph neural networks which can predict XPS with high accuracy for small-organic molecules overcoming computational challenges faced by traditional computational methods. We will also discuss the use of Koopmans' theorem for direct utilisation of Kohn-Sham eigenvalues as an input for our machine learning model for prediction using Δ-ML.[2]

References:

[1] P. Kayastha, S. Chakraborty and R. Ramakrishnan. (2022) Digital Discovery, 1, 689-702
[2] R Ramakrishnan, PO Dral, M Rupp, OA Von Lilienfeld (2015) Journal of chemical theory and computation 11 (5), 2087-2096

Friday, Mar 1st 2024

12:00 Hrs (Tea / Coffee 11:45 Hrs)

CR-1, TIFR-H