Title: Machine learning for high efficiency organic solar cell: A growing synergy

Abstract: Organic solar cell (OSC) has witnessed a rapid performance improvement due to the development of low band gap conjugated donors and novel A-DA'D-A non-fullerene acceptors (NFA) with efficiency reaching 19%. With excellent opto-electronic properties, the NFA molecules could achieve high open circuit voltage and current at the same time. Theoretical estimations showed that the efficiency of OSCs can be increased up to 21% if the energy loss can be reduced to lower than 0.4 eV. Designing asymmetric molecules with large dipole moments can bring significant improvement in this regard. To accelerate the discovery of functional organic semiconductors and rational device optimization, data-driven and experiment oriented machine learning (ML) approach could play crucial role. ML can provide an effective prediction model based on big data, avoiding the time-consuming high-throughput experiment. We have effectively predicted and screened the performance of OSCs based on various polymer:NFA combinations by employing a data-driven machine learning (ML) approach and successively validated the model by fabricating a set of highly efficient devices with a PCE up to 15.23%[1,2]. A dataset of 1242 experimentally verified donor:acceptor (D/A) combinations was constructed, and the corresponding material descriptors were generated to train and test five different supervised ML models for predicting the PCE, J_{SC} and V_{OC}. The proposed ML approach provides an effective method for predicting and virtual screening of donor-acceptor pairs with minimal energy loss and would be useful for developing next-generation high-performance solar cell materials.

References

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Short Bio:

Dr. Supravat Karak is currently working as an associate professor at the Department of Energy Science & Engineering, Indian Institute of Technology Delhi (DESE, IITD). Dr. Karak received his M. Sc. and PhD degree in Physics from Indian Institute of Technology Kharagpur. His broad research interest is to understand the fundamental photo-physics of several new class of polymer and hybrid materials and determining the performance limitation of the material in question with the aim to develop innovations that will lead to better device performance and higher device energy efficiencies. Prior to joining IIT Delhi, Dr. Karak worked in various international laboratories such as UMass Amherst (USA), and Nagoya University (Japan), and has contributed several original journal publications, patents and lecture presentations.

Dr. Supravat Karak

Recognition:

1. Visiting faculty, Nagoya University, Japan,
2. Early Career Research Award, SERB
3. JSPS Researcher Award, JAPAN
4. EFRC Fellowship, USA