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Predicting the Microstructure Stability in Photovoltaic Polymer-Fullerene Blends Using Figure of Merit*

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A theoretical understanding of the micro-structure of organic semiconducting polymers and blends is vital to further advance the optoelectronic device performance of organic electronics. We outline the theoretical framework of a combined numerical approach based on polymeric solution theory to study the microstructure of polymer-small-molecule blends. We feed the results of ab initio density functional theory quantum chemistry calculations into an artificial neural network for the determination of solubility parameters. These solubility parameters are used to calculate Flory–Huggings intermolecular parameters. We further show that the theoretical values are in line with experimentally determined data. On the basis of the Flory–Huggings parameters, we establish a figure of merit as a relative metric for assessing the phase diagrams of organic semiconducting blends in thin films. This is demonstrated for polymer-fullerene blend films on the basis of the prototypical polymers poly(3-hexylthiophene-2,5-diyl) (P3HT) and poly[(5,6-difluoro-2,1,3-benzothiadiazol-4,7-diyl)-alt-(3,3-di(2-octyldodecyl)-2,2,5,2;5,2-quaterthiophen-5,5-diyl)] (PffBT4T-2OD). After confirming the applicability of our model with a broader range of materials and differences in molecular weight, we suggest that this combined model should be able to inform design criteria and processing guidelines for existing and new high performance semiconducting blends for organic electronics applications with ideal and stable solid state morphology.

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