

# Digital Discovery

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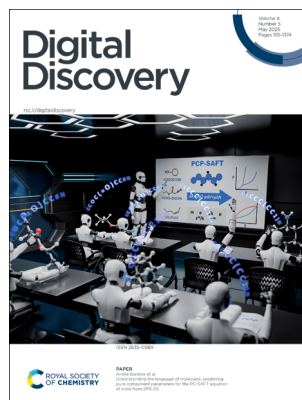
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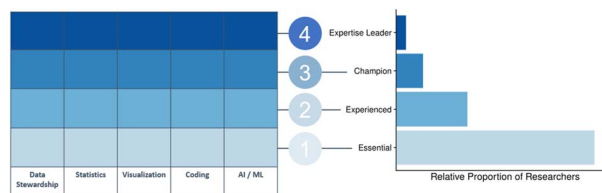
**Inside cover**  
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## PERSPECTIVE

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Mae V. Taylor, Zaid Muwaffak, Matthew R. Penny, Blanka R. Szulc, Steven Brown, Andy Merritt and Stephen T. Hilton\*



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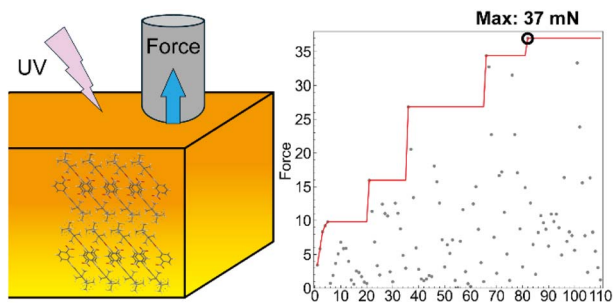
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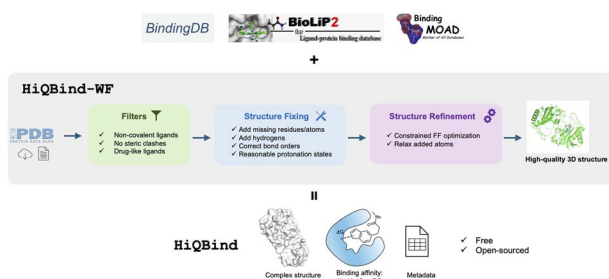
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### Machine learning-driven optimization of the output force in photo-actuated organic crystals

Kazuki Ishizaki, Toru Asahi and Takuya Taniguchi\*

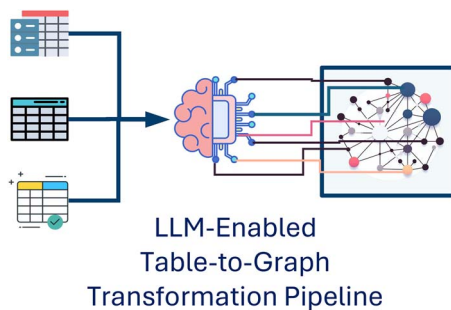
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### A workflow to create a high-quality protein–ligand binding dataset for training, validation, and prediction tasks

Yingze Wang, Kunyang Sun, Jie Li, Xingyi Guan, Oufan Zhang, Dorian Bagni, Yang Zhang, Heather A. Carlson and Teresa Head-Gordon\*

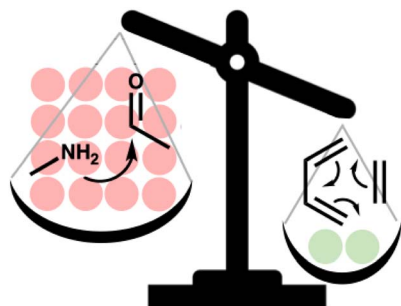
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Max Dreger,\* Kourosh Malek and Michael Eikertling

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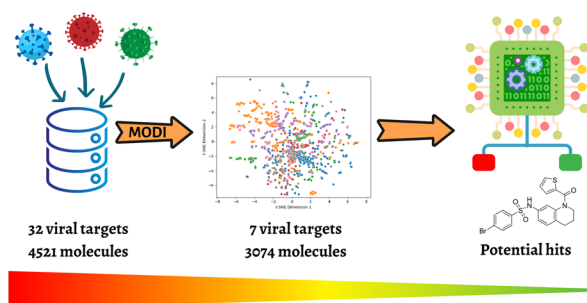
Angus Keto, Taicheng Guo, Nils Gönheimer, Xiangliang Zhang, Elizabeth H. Krenske and Olaf Wiest\*



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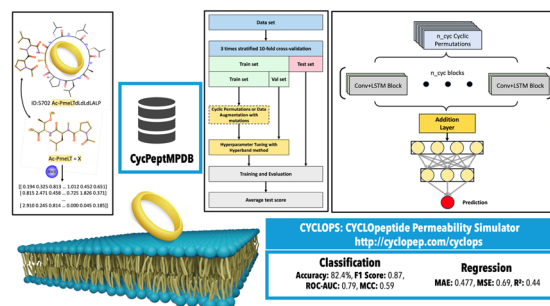
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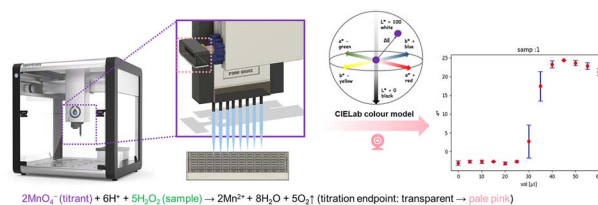
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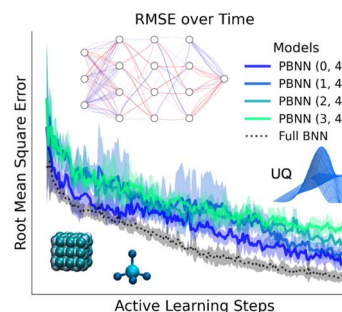
Yuan Li, Biplab Dutta, Qi Jie Yeow, Rob Clowes, Charlotte E. Boott\* and Andrew I. Cooper\*



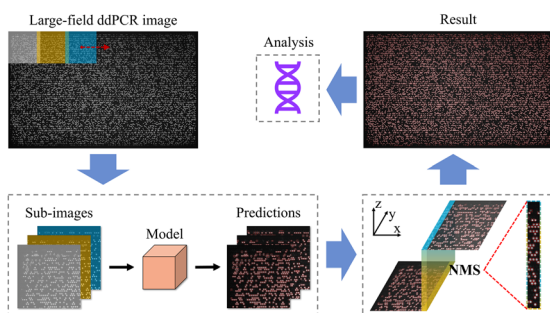
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## Active and transfer learning with partially Bayesian neural networks for materials and chemicals

Sarah I. Allec and Maxim Ziatdinov\*



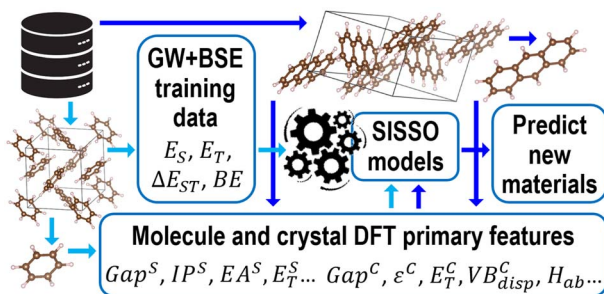
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Xingyu Jin, Jing Yang, Xiaorui Jiang, Zhenqing Li,\*  
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Dunlu Peng, Yoshinori Yamaguchi and Jijun Feng\*

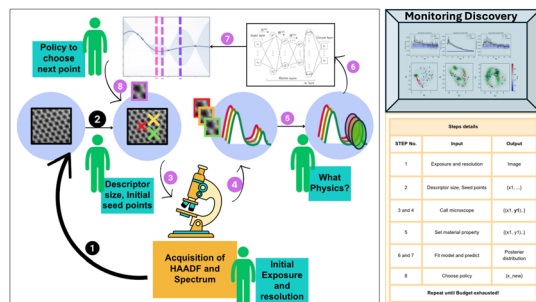
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### Predicting the excited-state properties of crystalline organic semiconductors using GW+BSE and machine learning

Siyu Gao, Yiqun Luo, Xingyu Liu and Noa Marom\*

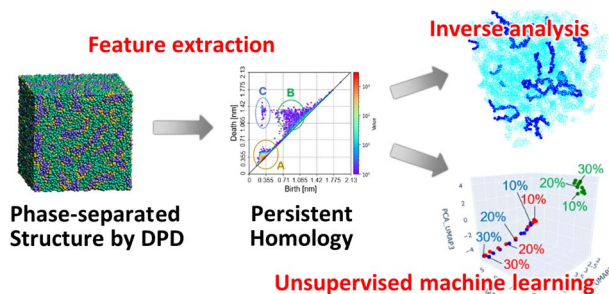
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Yukito Higashi, Koji Okuwaki, Yuji Mochizuki,  
Tsuyohiko Fujigaya\* and Koichiro Kato\*



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Armen G. Beck, Sanjay Iyer, Jonathan Fine and Gaurav Chopra\*

