

bot 5 materials

MCR-423

A1090B770

A1047B3

A1058B6





### Design Rules for Stable Organic Materials for Outer Space Solar Cell Applications

Andreas J. Bornschlegl<sup>1</sup>, J. Wu<sup>2</sup>, J. S. Rocha-Ortiz<sup>2</sup>, J. A. Posar<sup>3,4</sup>, A. J. Mozer<sup>5</sup>, L. Lüer<sup>1</sup>, C. J. Brabec<sup>1,2</sup>

- <sup>1</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute of Materials for Electronics and Energy Technology (i-MEET), Martensstraße 7, 91058 Erlangen, Germany
- <sup>2</sup>Helmholtz-Institute Erlangen-Nürnberg (HI-ERN), Immerwahrstraße 2, 91058 Erlangen, Germany
- <sup>3</sup>Sydney Nano Institute, University of Sydney, Camperdown, NSW, Australia <sup>4</sup>Future Industries Institute, University of South Australia, Mawson Lakes, SA, Australia <sup>5</sup>Intelligent Polymer Research Institute, Australian Institute for Innovative Materials, University of Wollongong, Wollongong, New South Wales 2522, Australia

### Motivation

- Find Radiation Hard Organic Materials
- Approximate space conditions in lab
- High-throughput screening of big material database
- Predict Gamma-ray stability from UVC stability



RMSE (train) = 0.406,

RMSE (test) = 0.432,

score(R2) = 0.631,

score(R2CV) = 0.454

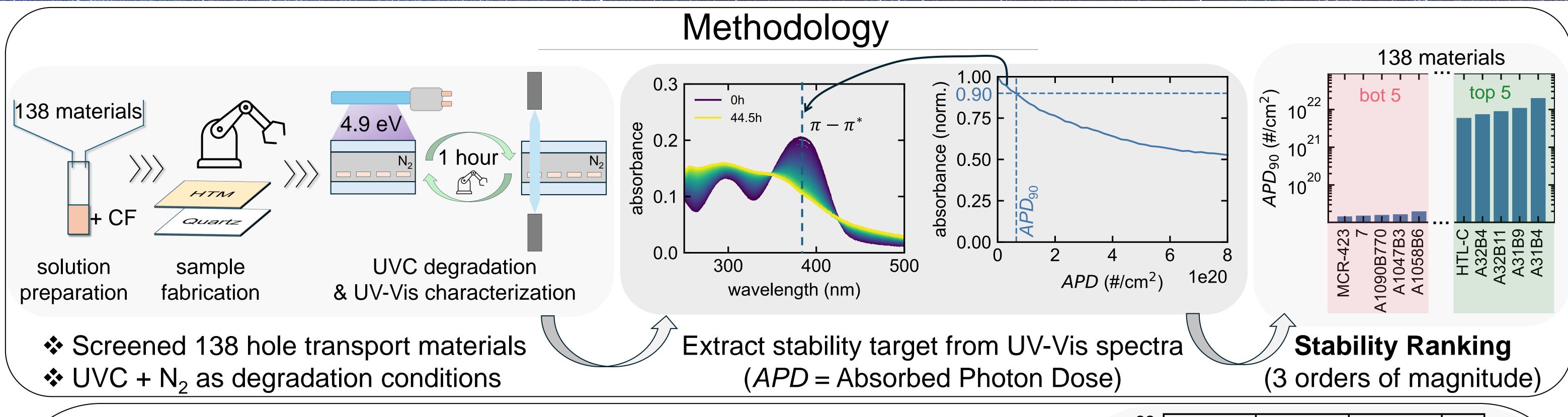
# fused ring clusters

20.5

20.0

19.5

8.0



Material Design Rules

top 5 materials

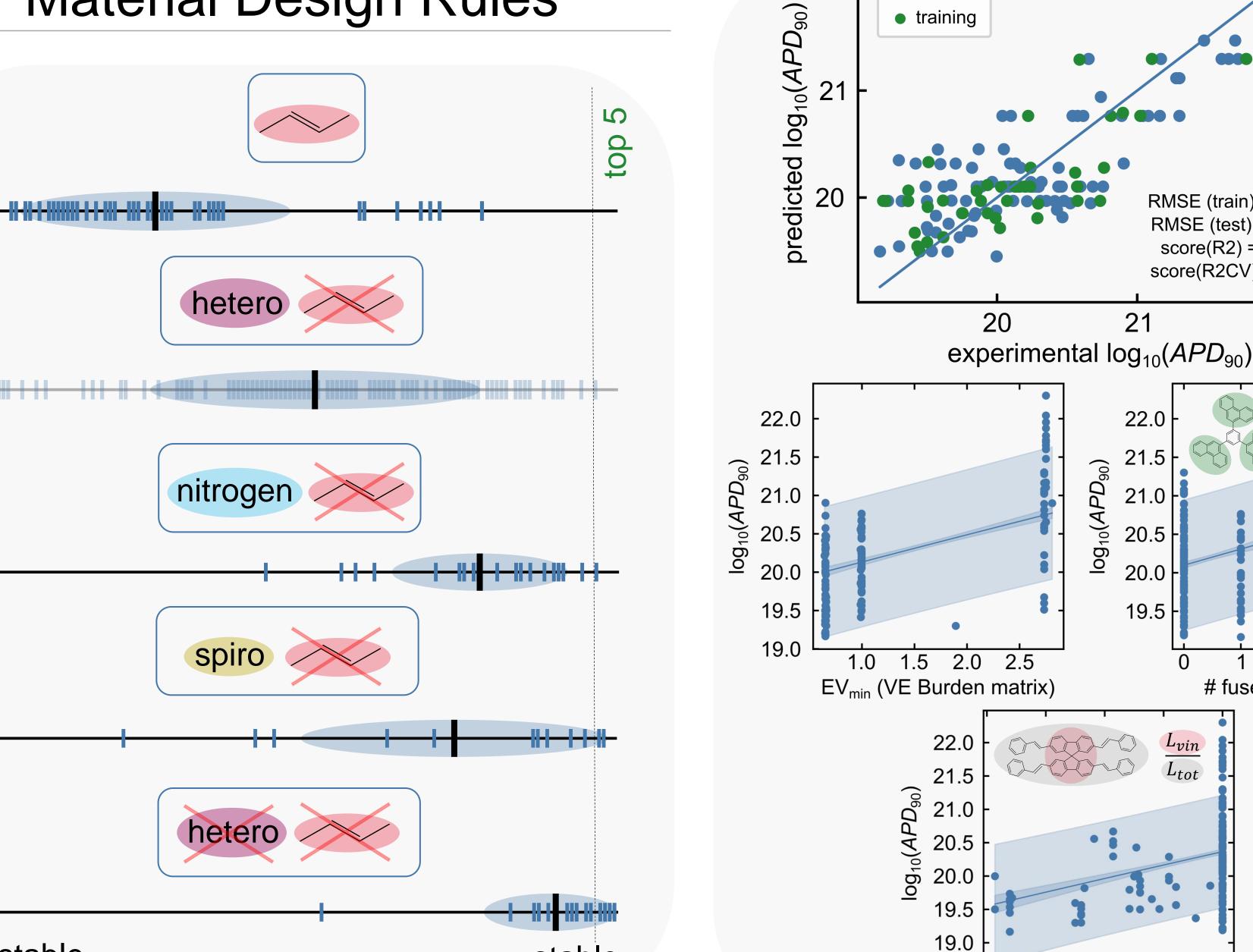
HTL-C

A32B11

A31B9

A31B4

stability



stable

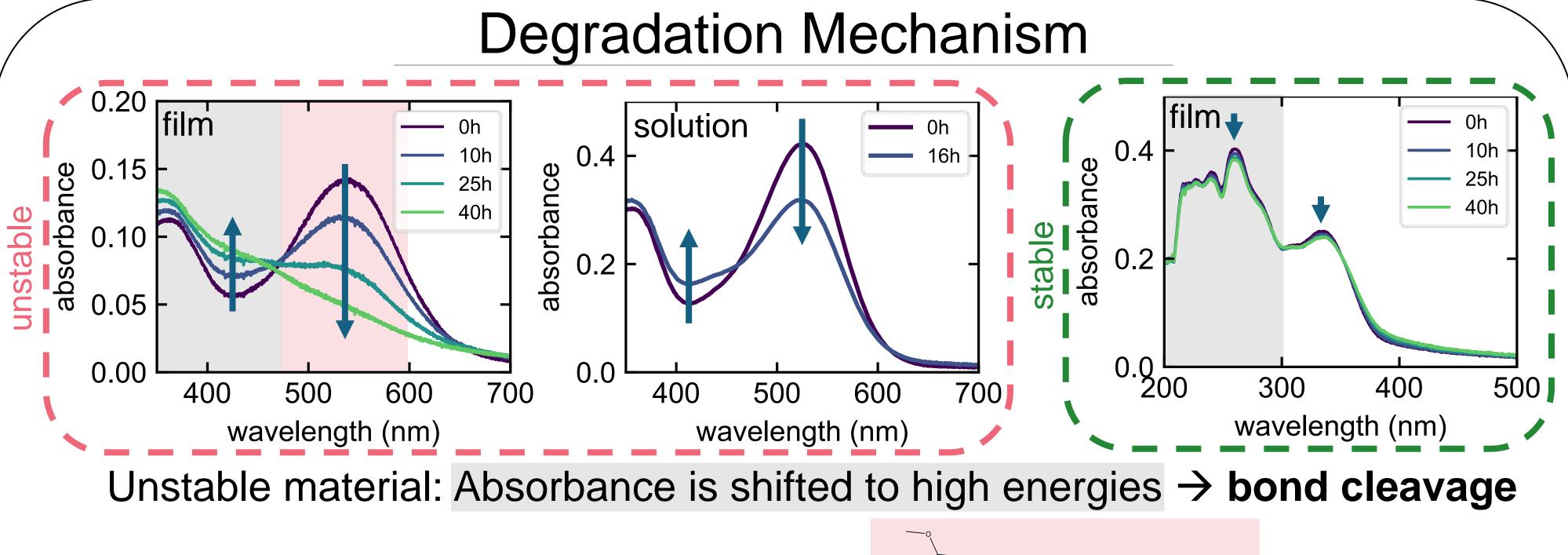
- High stability: Avoid heteroatoms & Vinylene
- Nitrogen atoms and spiro are acceptable
- Avoid Vinylene

test

Delocalization is important

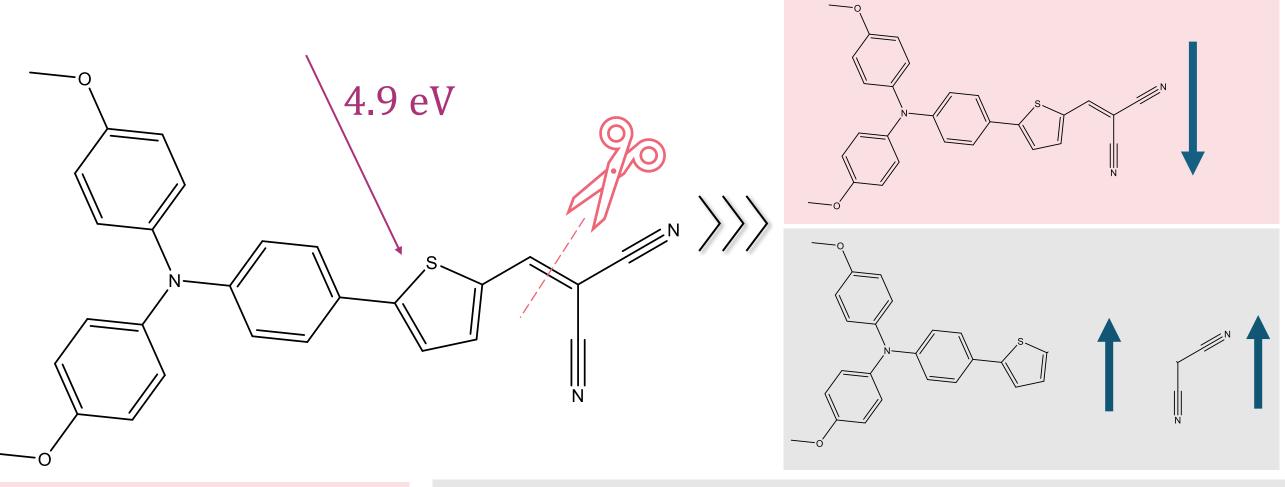
0.6

vinylene ratio



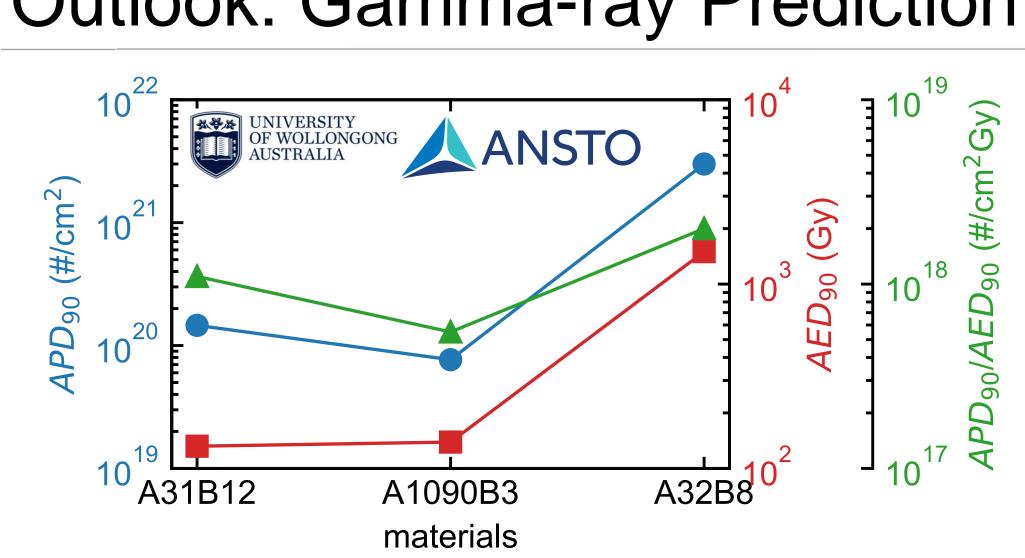
unstable

# 4.9 eV



When bond is broken, new molecules absorb at higher energies

## Outlook: Gamma-ray Prediction



- ❖ UVC has similar energy as Gamma 2<sup>nd</sup> e<sup>-</sup>
- Gamma and UVC stability have same trend
- Correlation factor doesn't differ much
- Results for 24 more materials soon

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Contact: andreas.bornschlegl@fau.de