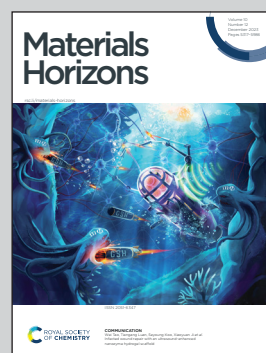


Showcasing research by Kazuo Takimiya and Kirill Bulgarevich
at RIKEN CEMS, Saitama and Tohoku University, Japan.

Crystal-structure simulation of molecular semiconductors:
brickwork-related crystal structures of methylthiolated
peri-condensed polycyclic aromatic hydrocarbons

Better than prediction by chance are novel computational
simulation methods for brickwork-related crystal structures,
which allow us to evaluate the likelihood of the appearance
of different polymorphs and to find new polymorphs
experimentally.

As featured in:



See Kirill Bulgarevich and
Kazuo Takimiya,
Mater. Horiz., 2023, **10**, 5492.