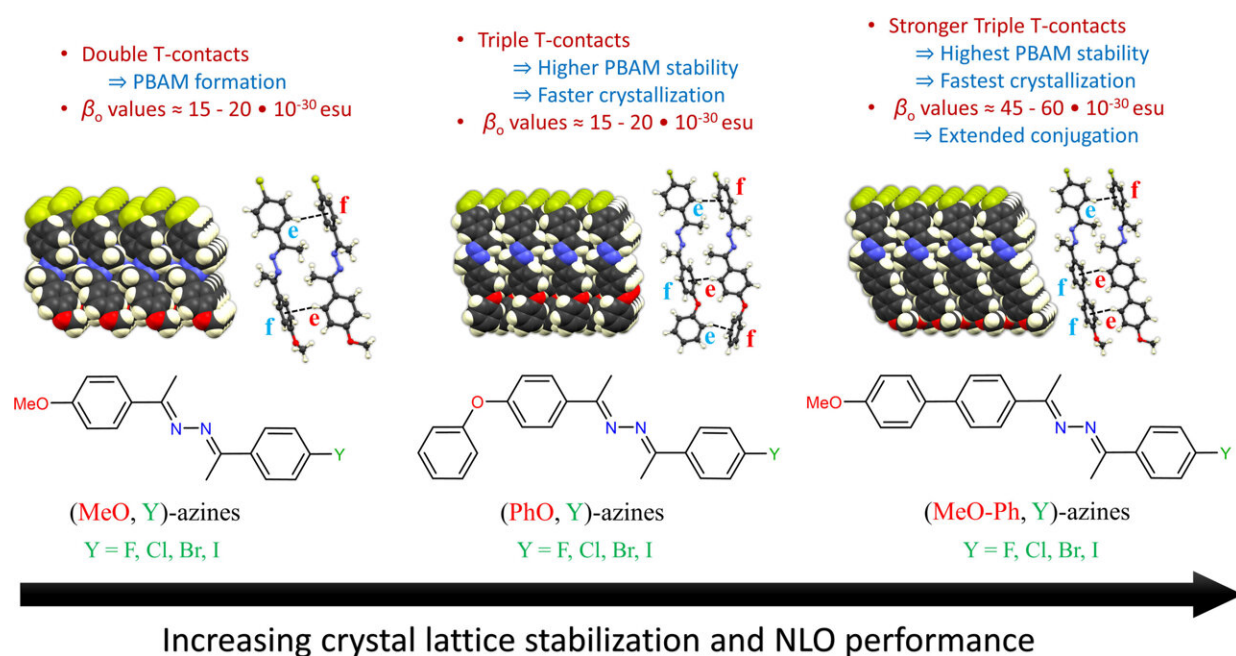


Researchers explore design of polar crystalline solids of pure molecular materials

August 30 2024, by Peter Ehrhard



Graphical abstract. Credit: *Chemistry – A European Journal* (2024). DOI: 10.1002/chem.202400182

Harmeet Bhoday, a Missouri S&T Ph.D. student in chemistry from Chandigarh, India, was the lead author of an article titled "Perfect Polar Alignment of Parallel Belamphiphile Layers: Improved Structural Design Bias Realized in Ferroelectric Crystals of the Novel Methoxyphenyl Series of Acetophenone Azines."

Journal editors selected the article as a [cover feature](#) of *Chemistry—A European Journal*. The research was also featured in "[Hot Topic: Crystal Engineering](#)."

Bhoday wrote the article with Dr. Nathan Knotts, a graduate of the University of Missouri, and Dr. Rainer Glaser, professor of chemistry at S&T.

"The focal point of our research has been the design of polar crystalline solids of pure molecular materials for [nonlinear optics](#)," says Bhoday. "Rather than merely seeking these crystals, we wanted to design organics and dipeptides that would want to crystallize with supramolecular architectures."

The team first tried to [design](#) molecules that would encourage strong lateral attractive interactions between side-by-side [molecules](#), but then discovered that they could go further and deliberately discourage the dipole antiparallel-alignment of polar materials for better performance. The research group has described the successful synthesis of four representatives of a new "methoxyphenyl series" of acetophenone azines.

"This study resulted in exciting insights about intra- and interlayer interactions," says Bhoday. "The interplay between intralayer and interlayer [intermolecular interactions](#) is challenging, and finding the right balance is permanently on our mind and the subject of extensive computational theorizing."

Bhoday says that thanks to the research, for the first time, it is now possible to establish experimental structure-function relations for the nonlinear optics activity of ferroelectric molecular crystals.

More information: Harmeet Bhoday et al, Perfect Polar Alignment of Parallel Bipoamphiphile Layers: Improved Structural Design Bias

Realized in Ferroelectric Crystals of the Novel "Methoxyphenyl Series of Acetophenone Azines", *Chemistry—A European Journal* (2024). [DOI: 10.1002/chem.202400182](https://doi.org/10.1002/chem.202400182)

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