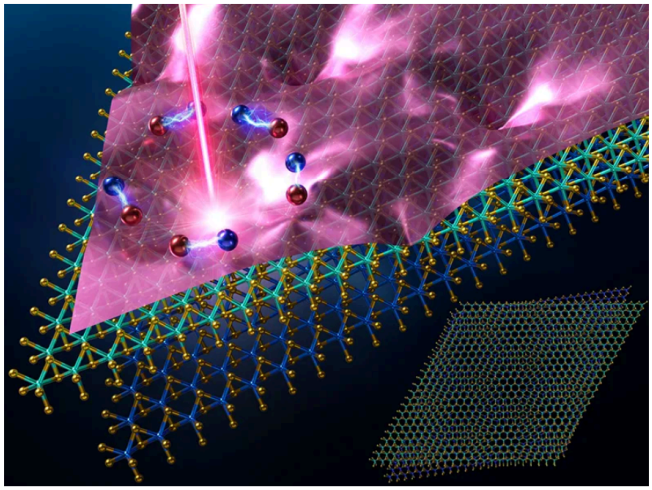
[Vol. 97] Reading Beyond the Peaks: MANA Study Finds Clarity in Spectral Complexity

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New method decodes hidden disorder in moiré materials from light-emission data



Title: Mapping the hidden disorder landscape of a moiré heterostructure
Caption: In a twisted $MoSe_2/WSe_2$ moiré heterostructure, photoluminescence varies from point to point as excitons respond to both smooth disorder and local trap-like sites. This illustration shows how spatial patterns in complex light emission can be used to infer a hidden hierarchical disorder landscape without assigning individual spectral peaks.
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A study from the Research Center for Materials Nanoarchitectonics (MANA), one of the centers under the National Institute for Materials Science (NIMS), presents a new method to decode hidden material disorder contained in complex photoluminescence spectra, paving the way for new optical diagnostics of material disorder in two-dimensional semiconductors and related light-emitting materials.

When two ultra-thin semiconductor layers, such as molybdenum diselenide and tungsten diselenide ($MoSe_2/WSe_2$), are stacked with a slight twist, they form a repeating pattern called a moiré heterostructure. These structures have unusual light-emitting properties, featuring a complex landscape of photoluminescence spectra across their surface. While scientists often analyze materials by looking at the individual peaks of their emission spectra, moiré heterostructures produce spectra with many overlapping peaks whose origins are difficult to explain individually.

To address this challenge, Katsunori Wakabayashi from MANA has developed a theoretical framework to explain this complexity. Rather than decomposing spectra peak by peak, his approach examines how simple descriptors, such as peak energy and average energy, change spatially across a sample.

By applying this theoretical framework to descriptor correlations reported for a $MoSe_2/WSe_2$ heterostructure, Wakabayashi found that different features respond to different layers of hidden disorder in the material, hinting at a hierarchy of disorder. The first level corresponds to a smooth 'background' that varies over larger distances of a few micrometers. In contrast, the second one is finer and much more localized, arising from small defects or exciton-trapping sites in the heterostructure. By comparing how these spectral features vary in space according to a detailed theoretical analysis, the underlying landscape of disorder in the bilayer material can be inferred mathematically without relying on spectral peak decomposition.

Tiny structural imperfections and hidden disorder can strongly affect how materials emit and interact with light. Thus, this new framework hints at a practical way to diagnose material quality issues directly from optical data, without relying on uncertain peak-by-peak spectral assignment. *This work could help researchers make better and more reproducible materials for light-emitting devices, optical sensors, and quantum technologies,"* remarks Wakabayashi.

References

Journal	Physical Review Research
Title	Hierarchical disorder in moiré exciton photoluminescence probed by spectral-descriptor correlations
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List of Research Highlights

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