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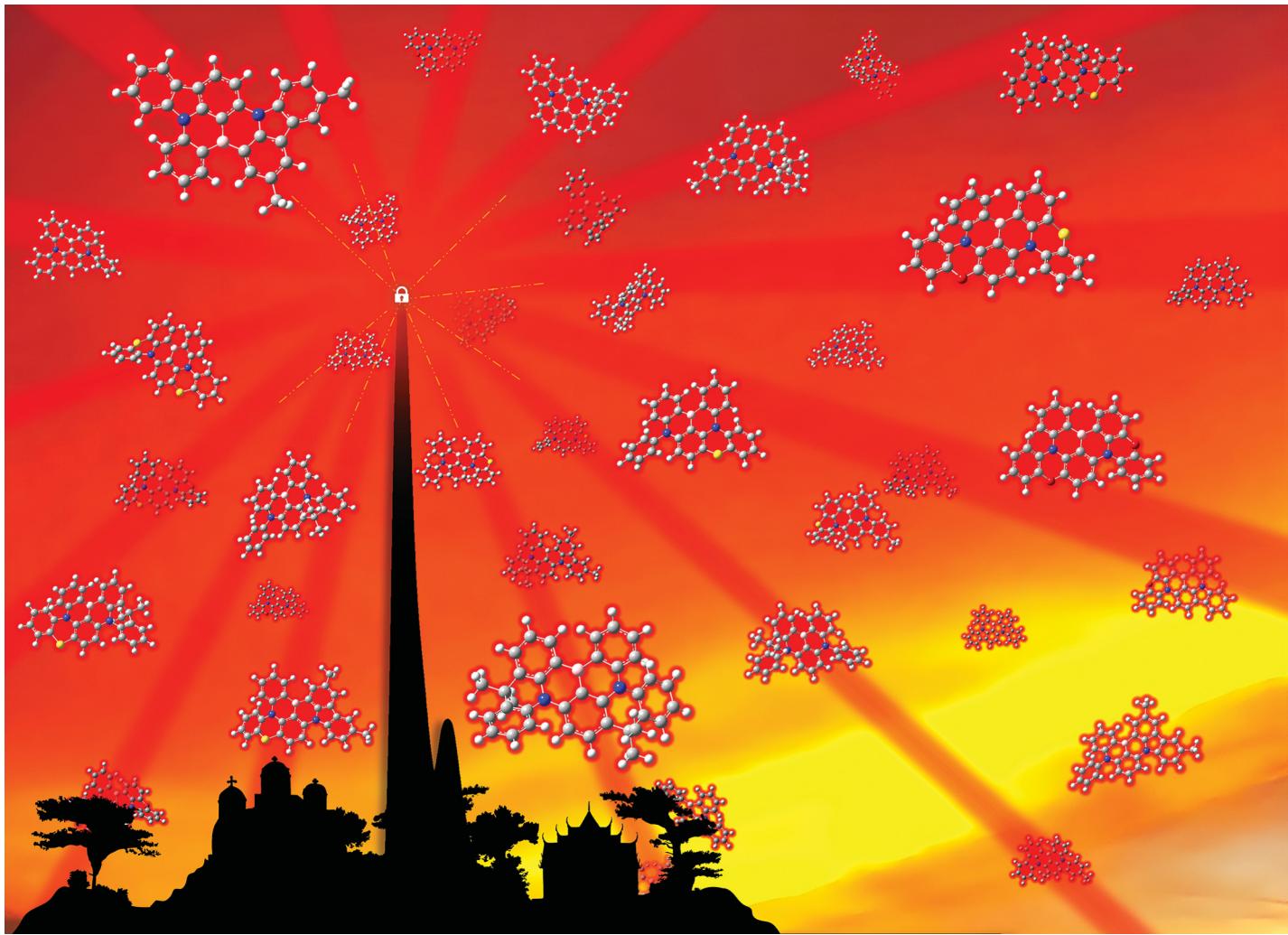
# Embracing research at the nexus of energy science and sustainability

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Fundamental questions  
Elemental answers

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Showcasing research from the Group of Prof. Chuan-Kui Wang, Prof. Lili Lin, and Dr Zhongjie Wang, School of Physics and Electronics, Shandong Normal University, China

Multi-resonance thermally activated delayed fluorescence molecules with intramolecular-lock: theoretical design and performance prediction

Multi-resonance thermally activated delayed fluorescence (MR-TADF) molecules with narrow full width at half maximum (FWHM) have attracted much attention recently. In this work, 36 borane/amine (B/N) type MR-TADF molecules were theoretically designed by using intramolecular-lock strategy and systematically studied based on first-principles calculations. It is found that intramolecular-lock is an efficient strategy for the design of highly efficient MR-TADF emitters.

### As featured in:



See Chuan-Kui Wang, Lili Lin,  
Zhongjie Wang et al.,  
*Phys. Chem. Chem. Phys.*,  
2023, **25**, 24406.