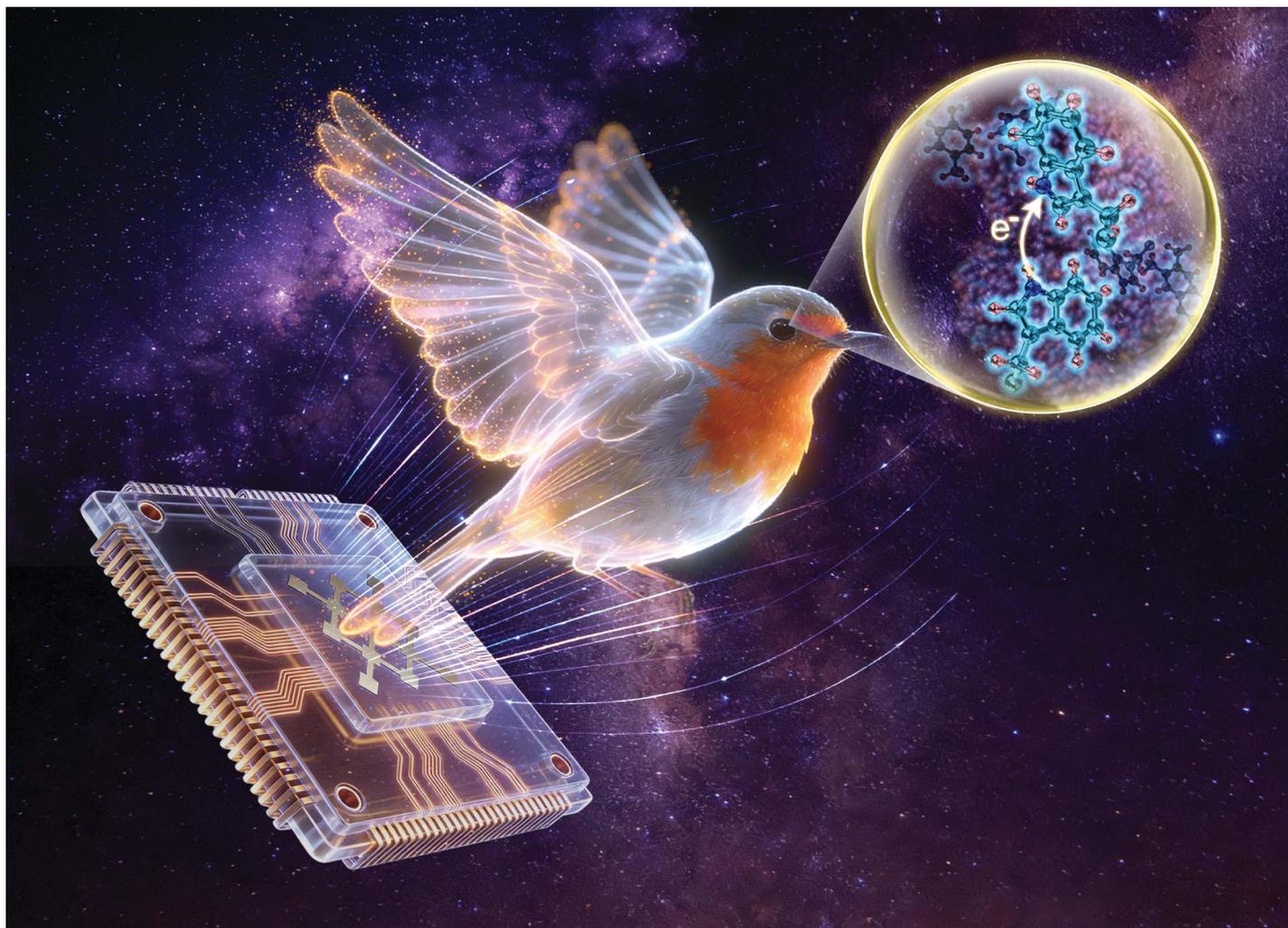


# EES Batteries

Exceptional research on  
batteries and energy storage

Part of the EES family

**Join** | Publish with us  
**in** | [rsc.li/EESBatteries](https://rsc.li/EESBatteries)



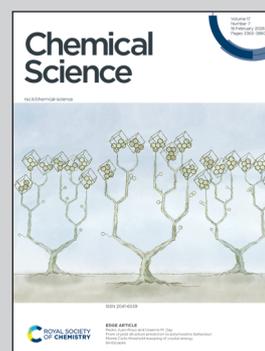
Showcasing research from Dr. Jun-Han Huang's group, BGI Research, Shenzhen, China and Prof. Weitang Li's group, School of Science and Engineering, The Chinese University of Hong Kong, Shenzhen, China.

Quantum-classical hybrid computation of electron transfer in a cryptochrome protein *via* VQE-PDFT and multiscale modeling

Accurate modeling of biological electron transfer is challenging due to complex electronic correlations. We present VQE-PDFT, a hybrid framework integrating active-space variational quantum eigensolver (VQE) with classical pair-density functional theory (PDFT) to efficiently recover both static and dynamic correlations. Applied to the cryptochrome protein ErCRY4 within a multiscale QM/MM architecture, this method yields transfer rates consistent with experimental spectroscopy. A demonstration on a superconducting quantum device further illustrates how this hybrid framework enables reliable biochemical predictions on near-term quantum hardware.

Image reproduced by permission of BGI Research from *Chem. Sci.*, 2026, **17**, 3492.

### As featured in:



See Jun-Han Huang,  
Yuxiang Li *et al.*,  
*Chem. Sci.*, 2026, **17**, 3492.