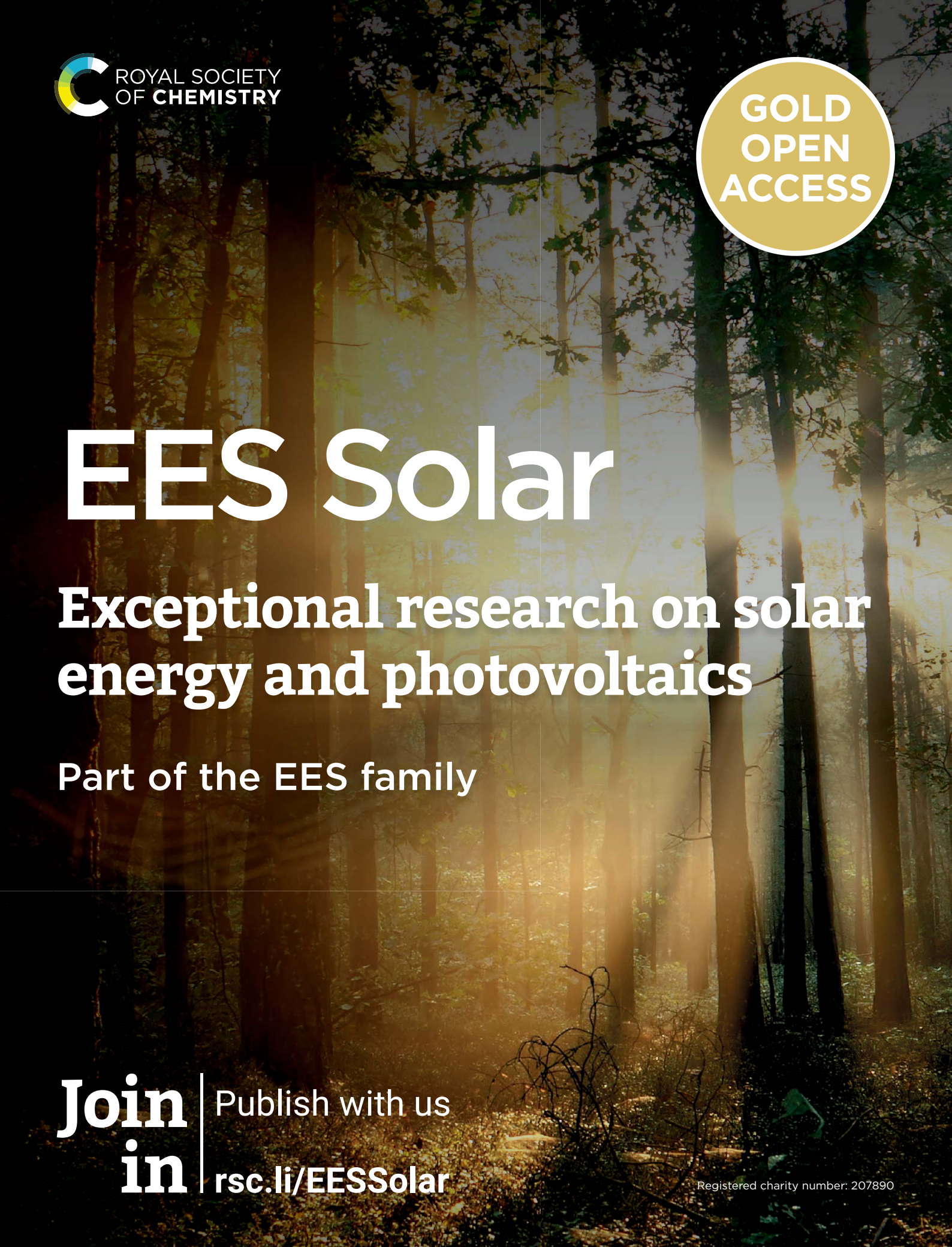
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A unified active learning framework for photosensitizer design

This work introduces a general and scalable active learning framework that streamlines molecular design workflows and substantially enhances exploration efficiency for chemists. By integrating machine learning calibrated computations, a large molecular dataset, and adaptive data acquisition, the framework accelerates the identification of promising candidates while reducing computational cost. The study demonstrates a broadly applicable approach for navigating vast chemical spaces and enabling more efficient, data-driven discovery in photochemical materials research.

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See Jiali Li, Rafael Gómez-Bombarelli, Aron Walsh, Xiaonan Wang *et al.*, *Chem. Sci.*, 2026, **17**, 916.

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