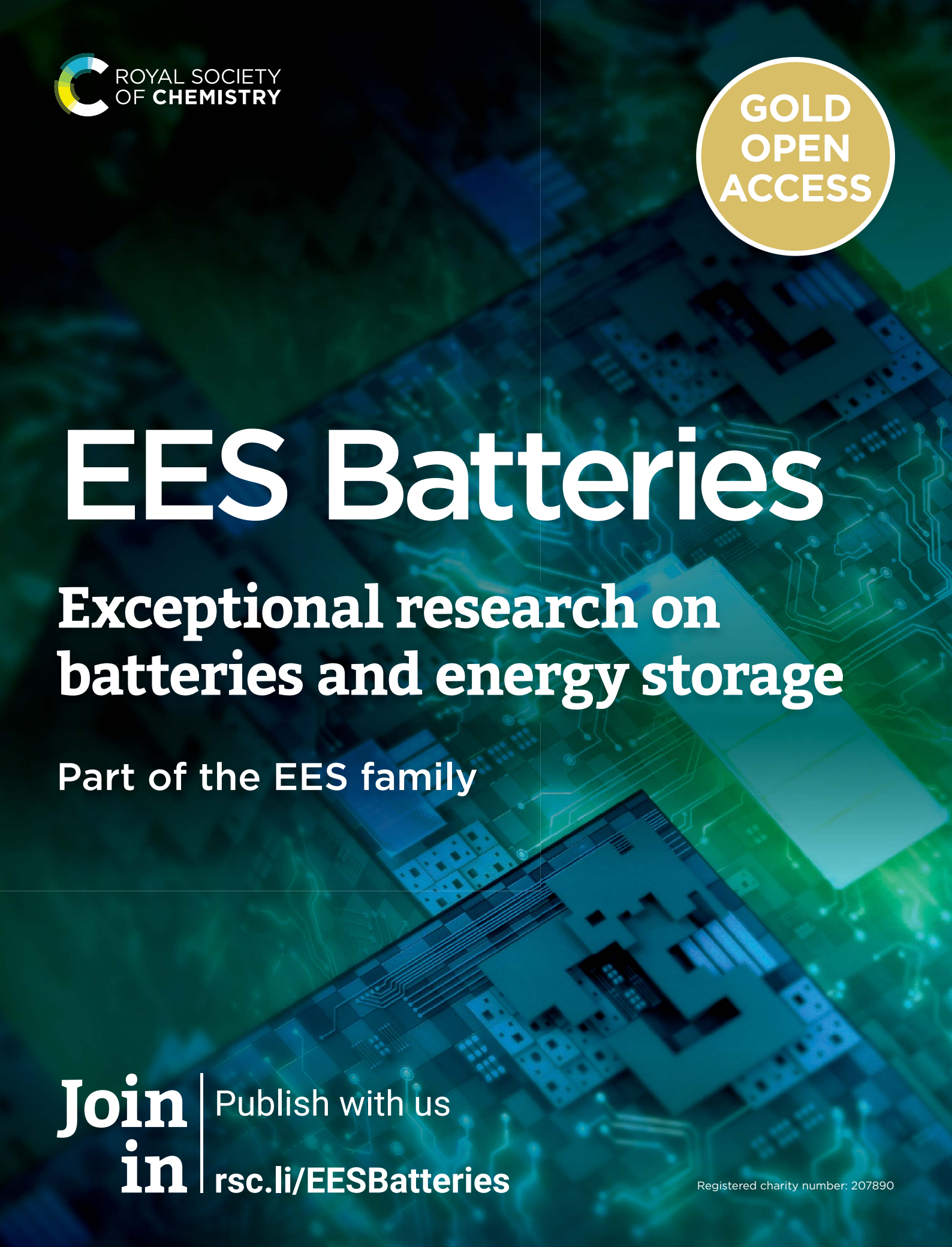
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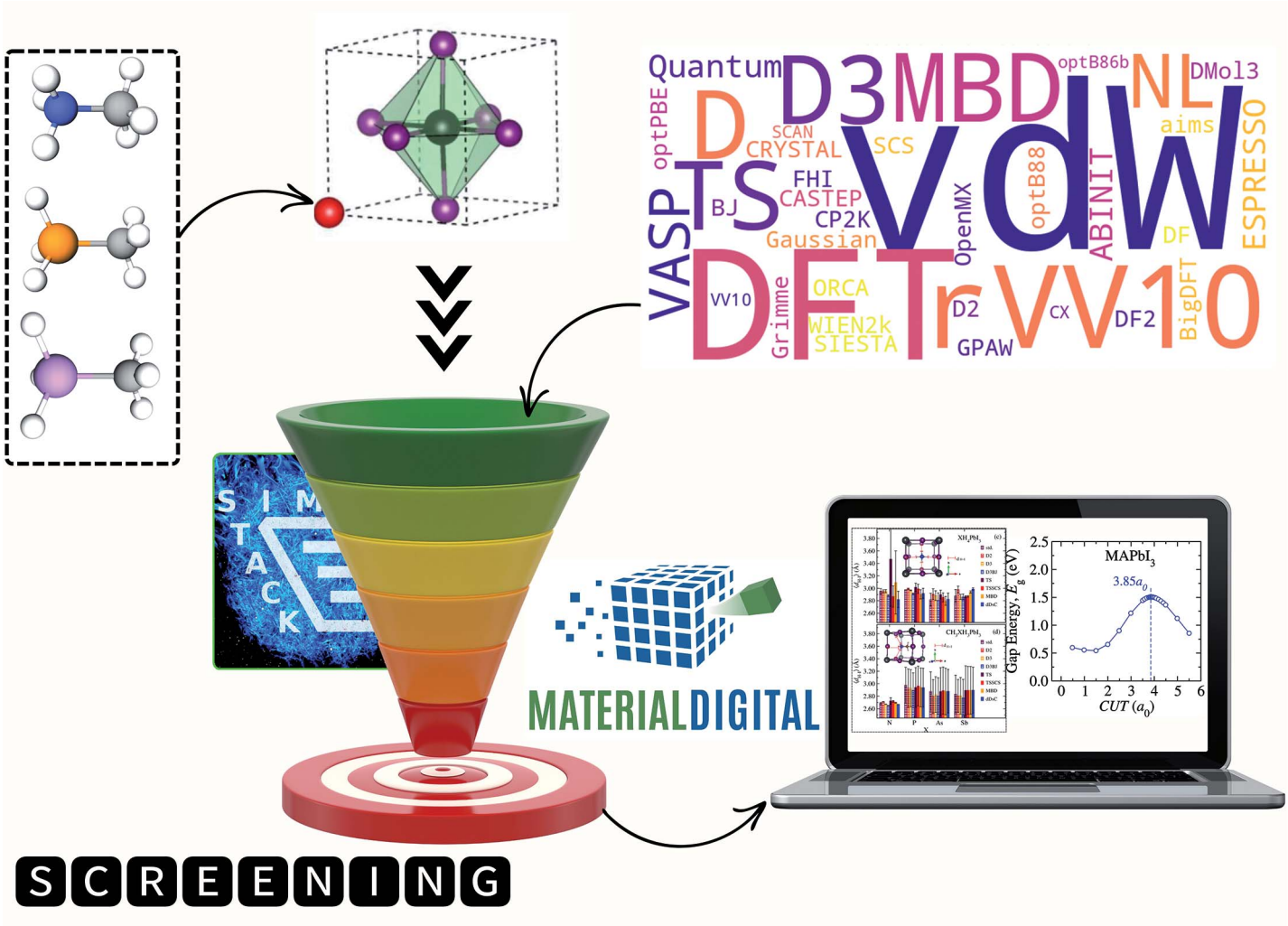

Showcasing research from Dr. Celso Ricardo Caldeira Rêgo, Institute of Nanotechnology and Platform MaterialDigital, Karlsruhe Institute of Technology, Germany.

Digital workflow optimization of van der Waals methods for improved halide perovskite solar materials

Hybrid organic–inorganic perovskites promise high efficiency at low cost but demand deeper insights into organic cation–inorganic interactions. Using a robust workflow powered by SimStack, we examine XH_4PbI_3 and $CH_3XH_3PbI_3$ (X = N, P, As, Sb) with DFT+vdW+SOC and DFT-1/2, uncovering critical impact of ionic radius and electronegativity on thermodynamic stability. This reveals how organic cation properties shift perovskite stability from NH_4PbI_3 toward Sb-based materials, opening pathways beyond $CH_3NH_3PbI_3$. This underscores workflow-driven efficiency in exploring next-generation perovskites.

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See Celso R. C. Rêgo *et al.*, *Digital Discovery*, 2025, **4**, 927.

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