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AI-guided stability design for perovskite photovoltaics

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Perovskite solar cells (PSCs) have entered a new phase where certified power conversion efficiencies (PCE) are now close to those of established photovoltaic technologies. However, the field remains bottlenecked by a more difficult question: can high performance survive realistic operational stress? Heat, illumination, bias, humidity, and outdoor exposure. These stresses rarely act on one layer alone but couple defects in the perovskite absorber, ion migration, selective contacts, buried interfaces, electrodes, and encapsulation. Stability is therefore a whole device-stack problem, not only a materials problem. The recent Science study by Guo and colleagues is significant because it mitigates this challenge through an AI-guided, system-level design route.[1] The authors report a p-i-n PSC with 25% efficiency and 97% of its initial performance after 1000 h of operation at 100°C under maximum power point tracking (MPPT). The device integrates $FA_{0.92}Cs_{0.08}PbI_3$ (FA is formamidinium) as the absorber, a UV-resistant carbazole phosphonic acid molecule, (4 ' -(3,6-dimethoxy-9H-carbazol-9-yl)-[1,1 ' -biphenyl]-4-yl)phosphonic acid (MeO-DPPACz), as the self-assembled (SAM) hole-selective layer, and bilateral ALD-Al_2O_3 layers as robust heterointerfaces. The performance is impressive, but the broader significance is methodological. The work shows how AI can connect literature knowledge, numerical modelling, molecular design, interface engineering, and stability testing across the full device.

AI FOR MATERIALS BEYOND MATERIALS SCREENING

This direction matters for "AI for Materials". General AI applications in materials research still focus on candidate selection: find a robust composition, molecule, additive, solvent, or processing condition that boosts one target performance. Such frameworks are useful, but perovskite photovoltaics require more than isolated prediction. A high-efficiency device can fail because of a weak SAM, unstable NiO_x contact, mobile ions, poor barrier layers, or a narrow processing window. Guo et al. move beyond single-component optimization by using a multi-agent AI framework (Figure 1). A data agent extracts and structures information from literature; a composition agent handles numerical modelling of FA-Cs-based perovskites; an interface agent analyzes contact layers and SAM design; a central agent coordinates the workflow and recommends device architectures. This structure is closer to a scientific decision system than a conventional screening model.

The first design target is the perovskite absorber. The central agent identified FA-Cs perovskite as a promising composition system, while the composition agent used Gaussian process regression (GPR) to refine the Cs-doping ratio. Instead of identifying common compositions such as $FA_{0.95}Cs_{0.05}PbI_3$ or $FA_{0.90}Cs_{0.10}PbI_3$, the framework pointed to $FA_{0.92}Cs_{0.08}PbI_3$. This choice was then validated through thermodynamically driven single-crystal growth, thin-film characterization, defect analysis, and device testing. The Cs8-based single crystal showed the lowest trap density, reduced dark current, lower hysteresis, strong PL uniformity, and positron annihilation results consistent with fewer vacancy-related defects. Thin-films based on this composition showed more uniform morphology, preferred orientation, and reduced trap-density. This chain links composition, thermodynamic stability, defect physics, and device aging in a way that a simple Cs-ratio screen would not. The single-crystal step is more than a characterization purpose. Thin-film

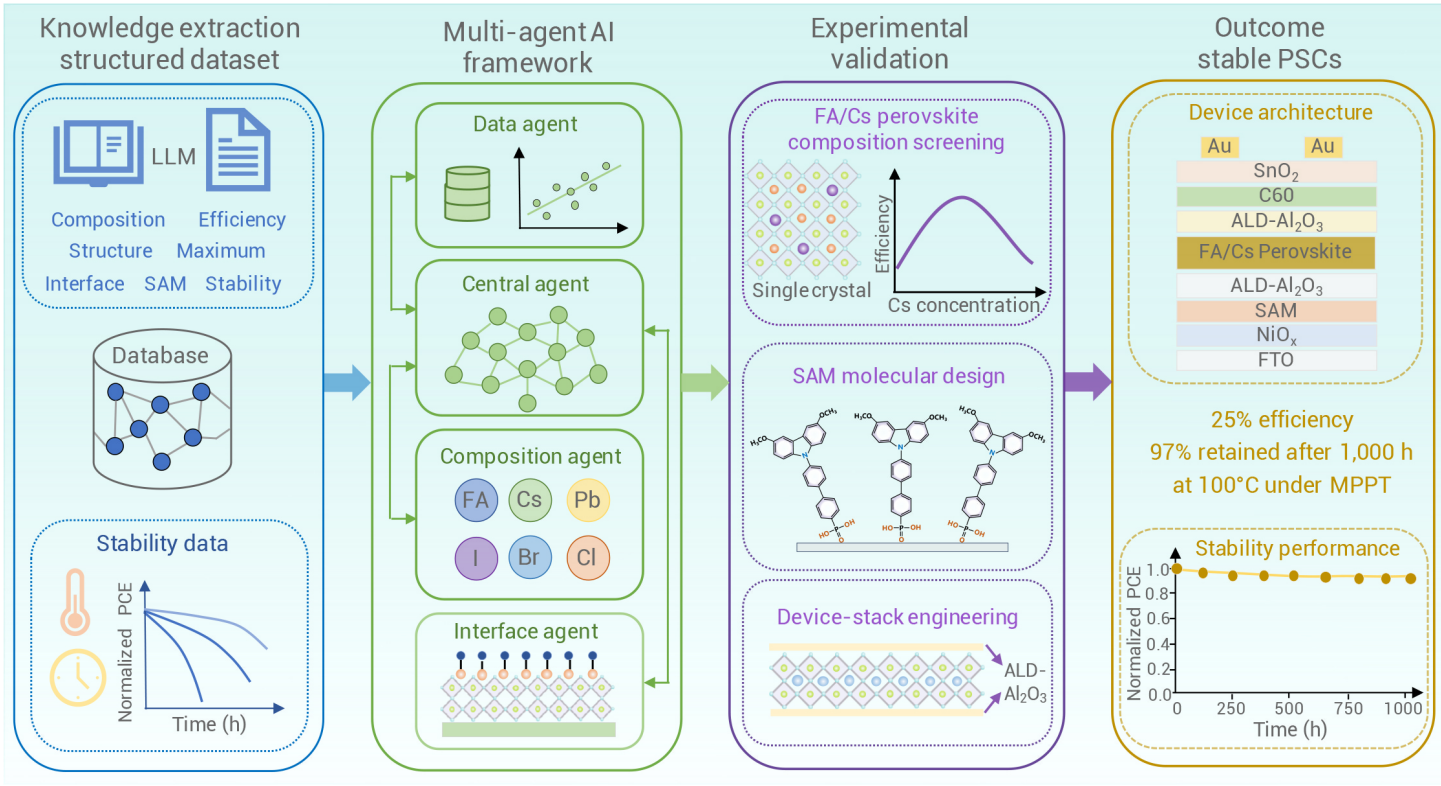

Figure 1. Workflow overview of a multiagent AI framework toward stable PSCs.

growth in perovskites depends strongly on precursor chemistry, solvent coordination, antisolvent quenching, intermediate phases, local drying kinetics, and annealing. These processes can entangle intrinsic composition trends. Single crystals provide a more thermodynamic reference for comparing FA-Cs compositions. This does not prove that the same composition will always be optimal under blade coating, slot-die coating, spray coating, or other scalable processes. It does, however, gives the composition choice a stronger physical basis than empirical film optimization alone.

The second design target is the molecular contact. SAMs are now central to high-efficiency p-i-n-structured PSCs, yet their long-term stability under heat and UV light remains a known weak point. The interface agent supported a design strategy based on stronger C-N bonds and extended conjugation. The alkyl group in [2-(3,6-dimethoxy-9H-carbazol-9-yl)ethyl] phosphonic acid (MeO-2PACz) was replaced with a biphenyl group and designed MeO-DPPACz. Calculations showed higher bond dissociation energy, while UV aging tests showed improved resistance to UV-induced degradation. The molecule also has a predicted dipole moment close to the range associated with efficient devices. UPS results further suggest favorable energy-level alignment on NiO_x. This part of the study shows how AI-assisted molecular design can be constrained by device-level needs, for example, UV stability, interfacial energetics, and hole extraction.

The third design target is the interface layer. The final architecture uses FTO/NiO_x/MeO-DPPACz/ALD-Al_2O_3/perovskite/ALD-Al_2O_3/C60/ALD-SnO_2/Au. In this configuration, ALD-NiO_x helps stabilize the SAM contact, while ALD-Al_2O_3 layers on both sides of the perovskite reduce interfacial defects, suppress ion migration, and provide internal stabilization. Under 100°C MPPT operation, the Cs8 device retains more than 97% of its initial PCE after 1000 h, while Cs4 and Cs12 controls drop below 50%. Cross-sectional SEM after aging shows compact grains in the Cs8 device, but voids and collapse in the controls. Damp-heat, outdoor stability, and third-party damp-heat tests further support the claim that the improvement is not limited to a single aging condition.

FROM AI PREDICTION TO SCIENTIFIC DECISION LOOPS

The broader lesson is that AI for perovskite photovoltaics should not stop at faster screening. The field needs AI systems that can connect unstructured literature, structured datasets, physical descriptors, experimental validation, and failure analysis.[2] Large language models (LLM) can organize scattered reports and generate hypotheses. GPR can guide composition search with uncertainty. XGBoost and molecular descriptors can help evaluate SAM properties. Yet none of these tools can establish device reliability on their own. They become useful only when coupled to synthesis, thin-film formation, microscopy, optoelectrical testing, and accelerated aging. The strength of this work is that these parts are linked in one decision chain.

At the same time, this approach highlights a major bottleneck for AI-driven photovoltaic research, that is data quality. Literature-derived datasets are valuable, but they are often incomplete and biased toward successful devices. Many reports lack key metadata, such as raw materials information, precursor age, substrate treatment, operation humidity, oxygen level, key processing parameter, thermal calibration, encapsulation, and preconditioning.[3] Stability metrics also vary across studies. AI agents trained on such data need metadata awareness, uncertainty labels, and data-quality flags. Otherwise, they may reproduce literature bias instead of producing transferable design rules.

CONNECTING AI-GUIDED DISCOVERY WITH MANUFACTURING

Manufacturing relevance should move to the center. The present work is a strong laboratory-scale demonstration, but commercial PSCs require scalable coating, module integration, encapsulation, and real-world durability. The same full-chain AI route could be extended to blade coating, slot-die coating, spray coating, inkjet printing, and roll-to-roll-compatible stacks. Self-driving platforms such as AMADAPs offer a laboratory-scale model for manufacturing-aware AI for materials by linking automated fabrication, high-throughput characterization, structured data collection, and ML-based decision-making loops.[4] In-line PL imaging, hyperspectral mapping, optical reflectance, thermal imaging, and electrical monitoring could provide real-time feedback during film formation and aging. Digital twins could link fluid flow, solvent evaporation, nucleation, crystal growth, defect formation, and device response. This would shift AI from recipe recommendation to wider-manufacturing-window discovery. In a word, several practical steps would help the field build on this work. Perovskite experiments need digital sample passports that record raw materials, precursor history, substrate treatment, deposition parameters, environment, annealing conditions, layer sequence, measurement settings, and aging protocol.[5] Benchmark datasets should include failed, average, and high-performing devices, not only champion cells. AI agents should be paired with in situ and operando probes because degradation pathways often appear only under combined stress. Design rules generated by AI should be tested across independent laboratories or platforms before broad claims of generality.

OUTLOOK: TOWARD SELF-IMPROVING PHOTOVOLTAIC RESEARCH

The authors do not solve every stability problem in perovskite photovoltaics, for example, the work does not yet establish module-level reliability, universal process transfer, or long-term outdoor durability across climates. It also leaves open the relative contribution of $FA_{0.92}Cs_{0.08}PbI_3$, MeO-DPPACz, ALD-Al_2O_3, processing conditions, and their interactions. These questions define the next experiments. The value of the study is that it reframes AI in emerging photovoltaics. AI should not be only a tool for faster materials screening, it can become an all-purpose way to organize scientific knowledge, coordinate device-stack decisions, and connect mechanisms with reliability tests. Perovskite photovoltaic technology will not reach real deployment through champion efficiencies alone. They need standardized data, reproducible protocols, robust process windows, cross-platform validation, and models that improve as new experiments enter the record. This work offers a clear step in that direction: a full-chain AI route from materials choice to stable device operation, and a blueprint for more self-improving photovoltaic research.

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DECLARATION OF INTERESTS

The author declares no competing interests.