AI-machine learning techniques applied to energy materials discovery and design

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Keywords: Machine learning, Density functional theory, Energy materials, Machine-learning interatomic potentials, Graph neural networks, Generative inverse design, Radioactive iodine adsorbents

The discovery and design of advanced materials for energy conversion and storage, as well as for the safe management of the nuclear fuel cycle, has traditionally relied on slow, intuition-driven cycles of synthesis and characterization. In this plenary lecture, I present how the convergence of quantum-mechanical computation and artificial intelligence/machine learning (AI/ML) is transforming this paradigm into a rapid, data-driven, and increasingly autonomous process, and illustrate the approach with our work on energy materials and on adsorbents for radioactive species.

At the core of our framework, machine-learning interatomic potentials trained on first-principles density functional theory (DFT) data accelerate atomistic simulations by several orders of magnitude, enabling high-throughput screening of vast compositional spaces. Graph neural networks serve as surrogate models that predict key properties—adsorption energies, formation energies, and selectivity—directly from atomic structure, while generative models combined with active learning enable the inverse design of candidate materials targeted at specified functions. Together these elements form a closed-loop discovery cycle in which AI-proposed candidates are validated by simulation and experiment, and the resulting data continuously refine the models.

As a representative application relevant to nuclear analytical science, I will describe reusable platinum-coated iron (Fe@Pt) core–shell nanoadsorbents for the selective removal of radioactive iodine (I^-, I_2, CH_3I, and ^{129}I) from complex aqueous media, achieving removal efficiencies above 99.8% and stable performance over 100 reuse cycles. DFT calculations revealed the atomistic origin of the selectivity—spontaneous chemisorption and dissociation of iodine into neutral atoms on Pt(111)—consistent with X-ray absorption, ICP-MS, GC-MS, and liquid-scintillation-counting measurements. This case demonstrates how mechanistic insight and AI-guided design jointly accelerate the development of high-performance materials, pointing toward autonomous laboratories for energy and environmental applications.

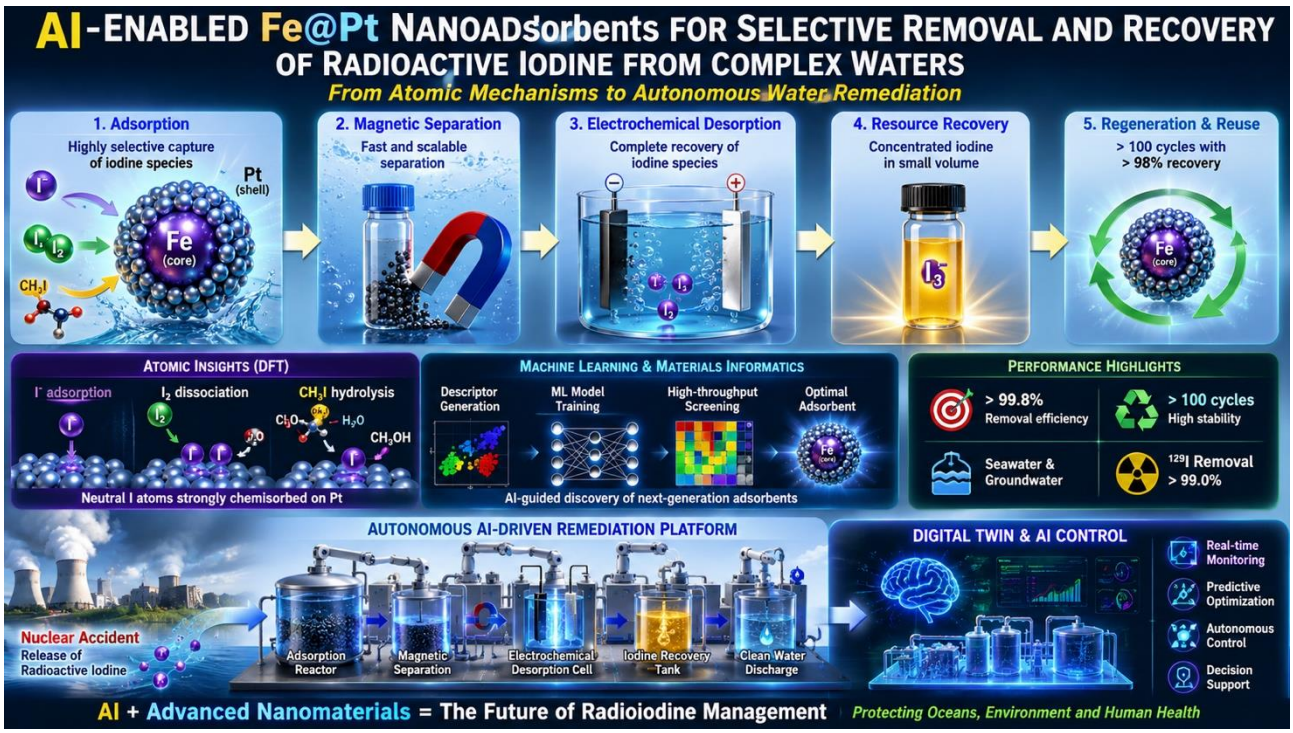

Fig. 1. AI/ML-driven closed-loop framework for energy materials discovery, illustrated by reusable Fe@Pt adsorbents for radioactive iodine: nuclear analytical characterization, first-principles DFT of iodine adsorption on Pt(111), and machine-learning design (ML interatomic potentials, graph neural networks, and generative inverse design). [image drawn with help of the ChatGPT]

Acknowledgement

This work was supported by This work was supported by the mid- and long-term nuclear research and development program (NRF-2017M2A8A5014716 and 2016M2B2B1945256) and by the Institute (2021M2E1A1085202) for Korea Spent Nuclear Fuel (iKSNF) and National Research Foundation of Korea (NRF) grant funded by the Korea government(Ministry of Science and ICT, MSIT). T. H. acknowledges financial support from the Research center Program of the IBS (IBS-R006-D1) in the Republic of Korea.