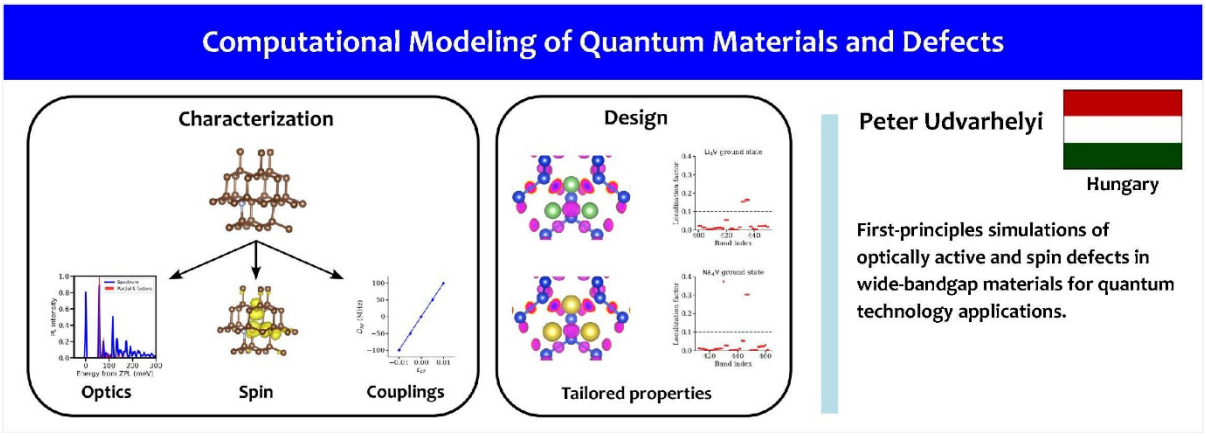
Computational Modeling of Quantum Materials and Defects

ICYS Research Fellow Dr. Peter UDVARHELYI



■Research

My research focuses on the theoretical and computational investigation of atomic-scale imperfections in solid-state materials, specifically, point defects that disrupt the periodic crystal lattice and give rise to localized quantum states. In wide-bandgap host materials, these defect states are energetically isolated deep within the bandgap, forming artificial atoms or molecules embedded in the crystal. These quantum systems, known as color centers and spin defects, can be coherently manipulated, making them foundational elements for emerging quantum technologies such as quantum communication and sensing. Using first-principles calculations, I explore their formation energies, optical transitions, and magnetic properties, providing essential insight for tight experimental control. Beyond defect structure identification and characterization, I investigate how external perturbations affect their properties, and I explore how these couplings can be harnessed for precision sensing and dynamic tuning. A key goal is the theoretical design of novel quantum defects with tailored properties for specific applications. My work intersects condensed matter physics, quantum optics, and materials science, and benefits from close collaboration with experimentalists specializing in crystal growth, ion implantation, and advanced spectroscopy.

■Comments

I am originally from Hungary, where I earned my Ph.D. in Physics. Following this, I spent three years conducting postdoctoral research in Hungary and an additional year and a half in the United States. These experiences deepened my expertise and broadened my perspective on international scientific collaboration. Currently, I am embarking on my independent research career at ICYS within NIMS, a unique environment that provides both the foundational resources and intellectual freedom essential for early-career scientists. ICYS fosters a truly interdisciplinary ecosystem where theoretical modeling, advanced fabrication techniques, and state-of-the-art characterization methods converge to accelerate materials innovation. What sets ICYS apart is its vibrant multicultural community. Researchers from diverse national and academic backgrounds come together here, creating a dynamic space for sharing ideas, collaborative problem-solving, and mutual learning.

■Link

https://www.nims.go.jp/icys/research/#UDVARHELYI