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As a computational physicist, I perform first-principles calculations based on density functional theory in my research investigations to understand properties of materials and related processes in the atomic scale. My research studies are focused on the interactions of atoms and molecules with metal surfaces and two-dimensional materials.

The depleting supply of conventional fossil fuels and their impact on the environment during combustion serve as my motivation in my research activities. When I was a graduate student in Japan, I was involved in designing hydrogen electrodes for hydrogen-based fuel cells in collaboration with Toyota Motor Corporation and automotive exhaust catalyst for diesel engine vehicles in collaboration with Daihatsu Motor Co., Ltd. These studies encouraged me to perform investigations that will further improve the stability and performance of low-cost transition metals as catalysts for various reactions.

At present, my group is working on the modification of the electronic properties of low-cost transition metals to tune their reactivity and qualify them as catalysts for reactions involving

greenhouse gases, including carbon dioxide and carbon monoxide. Further, we are exploring potential materials for hydrogen separation membranes with reduced precious metal loading. The work aims to reduce the cost of hydrogen production and purification with agricultural wastes as the source. I collaborate with experimentalists to verify the computational results and to materialize the designed catalysts.

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