

KASAI LAB

[Designer Materials Realizing Quantum Technologies]

Guest Chair for Advanced Interdisciplinary Modeling

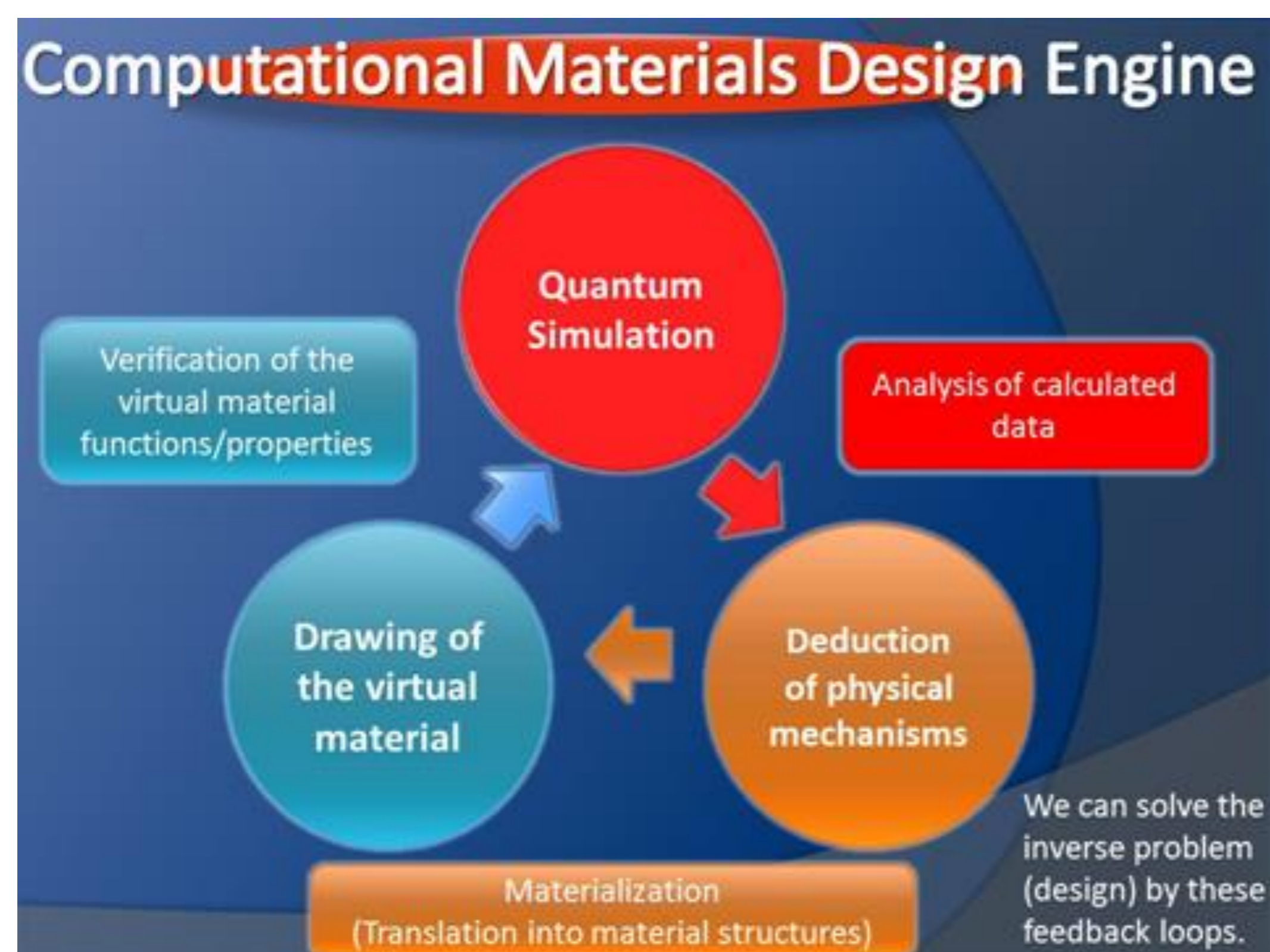
http://oflab.iis.u-tokyo.ac.jp/Main/Kasai_index.html

Computational Material Design

Designer Materials Realizing Quantum Technologies

Introduction

The Guest Chair for Advanced Interdisciplinary Modeling was established to research phenomena occurring in materials at the atomic levels. It aims to elucidate/control/design physical properties by investigating dynamical quantum processes in various reactions especially at surfaces, interfaces, carbon materials, and organic molecules. The results are widely applied in quantum devices such as fuel cells, spintronics, and solar cells, and recently in medical fields related to bio-sensors, photodynamic therapy, depigmentation therapy, and anti-tumor treatment. The group strongly believes that a universal understanding of these physical occurrences in materials is significant in order to unravel the challenging mysteries of this physical universe.



Actual achievements of our R&D

Case 1: Catalysis	Case 2: Hydrogen Storage
<p>Catalysis for vehicle emission control</p> <p>Understanding conventional catalysis of noble metals.</p> <p>CMD-Naniwa</p> <p>High-performance new catalyst design</p> <p>Ex. NOx reduction catalysis → designed new NO dissociative adsorption surface</p> <p>JP Patent No. 5002761, 15 other patents and more than 20 academic papers.</p>	<p>Understanding quantum states of hydrogen in materials</p> <p>CMD-Naniwa</p> <p>New invention for hydrogen storage system</p> <p>JP Patent No. 4222932, 7 other patents and more than 20 academic papers.</p>

Actual achievements of our R&D

Case 3: Fuel Cell	Case 4: Resistive Random-Access Memory
<p>Understanding the various elementary reactions in Fuel Cell by CMD-Naniwa</p> <ul style="list-style-type: none"> Analyze obstructive factor How to reduce the deterrent factors Finding the rate-controlling step → design alternative reactions with higher-active catalysis <p>CMD-Naniwa</p> <p>Ex. Dissociative adsorption of oxygen molecules on Pt surface → New designed surface</p> <p>JP Patent No. 3765050, 12 other patents and more than 30 academic papers.</p>	<p>Development of the next generation non-volatile RAM</p> <p>CMD</p> <ul style="list-style-type: none"> Voltage pulses can induce the transition between high- and low-resistivity states clarification of the mechanism of formation of the conduction channel <p>Press release : Sep. 2011</p> <p>JP Patent application No. 2006-257970/355977, 3 others and more than 10 academic papers.</p>

CMD-driven creation of new technology and next generation industries

