

CMD WORKSHOP – OSAKA

September 1 – 5, 2025

***Introductory Lecture
on
Computational Materials Design***

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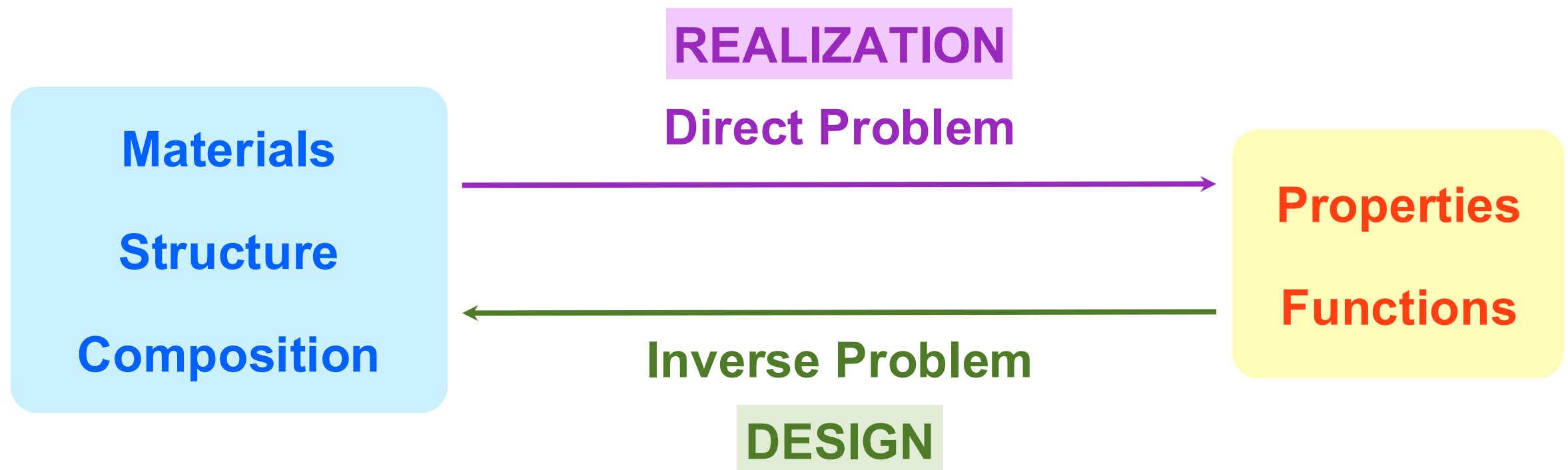
OUTLINE

- **Materials Design**
- **Computational Materials Design: CMD[®]**
- **History of the CMD[®] Workshop**
- **First-Principles Calculations**
- **Special Features of the Present CMD[®] Workshop**

CMD[®] is a registered mark by the CMD[®] consortium.

Materials Design

- **Goal of Materials Design**
 - **Discovery of novel materials with desired property/function, generally including optimization of property/function that known materials already possess**
- **An Inverse Problem of Realization**



Computational Materials Design: CMD[®]

- **CMD[®] is the theoretical design/optimization of materials with desired property/function. Specifically, CMD[®] involves the efficient use of computational techniques to conduct calculations based on the basic quantum theory.**
- **Key Developments of Emerging CMD[®]**
 - **Quantum Theory of Electrons**
 - **Electronic states governing most of properties (and often functions) that materials possess**
 - **Computational Techniques: Methods, Algorithms, and Codes**
 - **High-Performance Computers**
- **The purpose of the CMD[®] Workshop is to provide the fundamental knowledge and techniques needed to enable materials design by computations.**

スーパーコンピューター Top500



Computer exceeds Human Brain?

- Yes in chess in 1997
- Yes in Japanese chess in 2013
- Yes in games of go in 2016.



Computational Materials Design Workshop

- **Background**
 - **In 2001-2002, a Specialist Training Project was held at the International Institute for Advanced Studies (IIAS) in Kyoto, in the field of Information Biology. — An active effort to not merely ensure that the students acquired the target knowledge but rather to create opportunities for bilateral interchange with the instructors, with the aim of using the synergy to train a group of specialists who would become the future leaders in these areas.**
 - **Osaka University had many researchers specializing in first-principles calculations: Profs. H. Akai, H. Katayama-Yoshida, H. Kasai, and so on. They launched the “Development of methods for computational nano-materials design” computer-based project involving some other researchers in Japan under the support of JST in 2001.**
 - **Through the receipt of assistance from the JST project, the CMD[®] Workshop was born in September 2002 as the second IIAS specialist training project.**

1st CMD[®] Workshop at IIAS in September 2002



コンピュータ・マテリアルズ・デザイン ワークショップ 於 国際高等研究所 平成14年9月18日(木)

↑
Morikawa

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Yoshida

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Akai Kasai

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Hamada

↑
Nakanishi

Computational Materials Design Workshop

- **Since 2002 the 5-day Workshops have been held twice a year (spring and autumn) and the 47th Workshop is held here.**
 - **Total number of participants (till 46th WS): 2,253**
 - **Grad. & Undergrad. Students: 1,381**
 - **University/College Staffs (incl. National Labs): 305**
 - **Industry Researchers: 567**

<https://cmdworkshop.sakura.ne.jp/former.html>

Asian CMD[®] Workshop

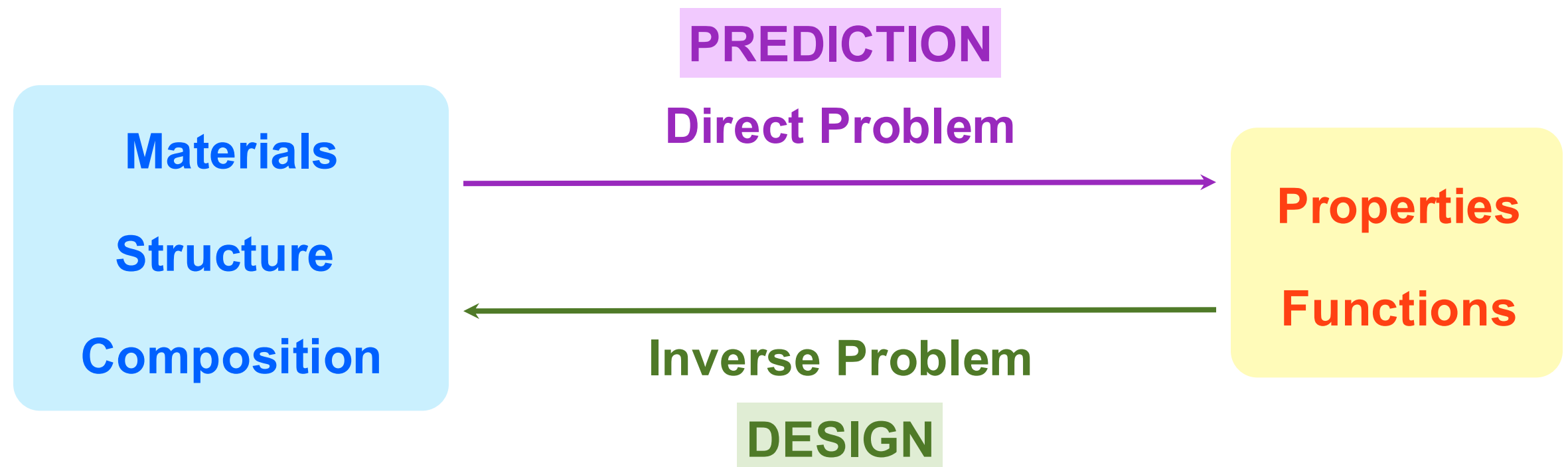
- **Since around 2007, the number of foreigners attending the Workshop from Southeast Asia has increased. Most of these are graduate students studying abroad at Osaka University. This made it difficult to conduct the lectures and hands-on training in Japanese only, and not only the explanatory slides but the oral explanations came to be presented in both Japanese and English. This style of instruction has continued to these days, but it has produced problems as well.**
- **Interchange with people from the Southeast Asian region through the CMD[®] Workshop became the inspiration in 2008 for the start of Asian CMD[®] Workshop in Southeast Asia. In August 2008, the first Asian CMD[®] Workshop was held at Institut Teknologi Bandung in Indonesia. In September 2008, an Asian CMD[®] Workshop was held at De La Salle University in the Philippines. In the following year, Asian CMD[®] Workshops were held again in Indonesia and the Philippines, and in Vietnam as well. In 2010, the number of countries was expanded to four with the addition of Thailand. It has continued to be held till these days.**

4th CMD[®] Workshop at DLSU in 2011



First-Principles Calculations

- Provide a way for solving a direct problem by prediction.



First-Principles Calculations

- ★ *Starting from first principles, equations are derived under some approximations and solved for a realistic system.*
- ★ *Two main characteristics:*
 - **General-purpose**: the methods do not depend on material systems and properties to be studied
 - **Non-empirical**: the methods do not require any experimental parameters and knowledges as input except for fundamental physical quantities (m , e , h)
- ▶ We may possibly:
 - Predict properties to be compared with experiments
 - Understand underlying microscopic mechanisms
 - Design new materials with desired property/function

First-Principles Calculations

- **Basic Approximations**
 - **Born-Oppenheimer Approx. → Interacting N-electron problem under external field (nuclear position: structure)**
 - **One-electron Approx. → Non-interacting problem**
 - **Local Density Approximation to Density Functional Theory**
→ **Kohn-Sham equations to be solved**
- **Band Theory for Crystalline Systems**
- **Real-Space Methods for Nanostructure Systems**

What We Get

- Many kinds of physical quantities that can be directly compared with experimental observables
 - *Structural properties*
 - heat of formation, phonon, elastic constants, thermal expansion, ...
 - *Electric properties*
 - electric polarization, piezoelectric constants, Born charges, ...
 - *Magnetic properties*
 - magnetic moments (spin and orbital), magnetic coupling, magnetoanisotropy energy, hyperfine constants, ...
 - *Optical properties*
 - optical constants, absorption spectra, ...
 -

46th CMD[®] Workshop

- **Beginners Course**
 - **ABCAP, Machikaneyama, STATE-Senri**
- **Advanced Course**
 - **HiLAPW, RSPACE, FPSEID²¹**
 - **Machikaneyama, Naniwa-Series, Salmon**
- **Supercomputer Course**
 - **STATE-Senri**
- **Expert Course**
- **Spintronics Design Course**
- **Lectures**
 - **Three lectures on CMD Studies**
 - **Daniel Packwood, Fumiyuki Ishii, and Shoji Ishibashi**

Hope you enjoy the Workshop

[**https://cmdworkshop.sakura.ne.jp**](https://cmdworkshop.sakura.ne.jp)