Report to 2023 APDIC

Activities in 2023 Korean Committee of Computational Materials Science and Engineering

May 31, 2024

In-Ho Jung

Korea Institute of Metals and Materials (KIMM)

- Two divisions in KIMM
 - Computational Materials Science Division (over 25 years)
 - Artificial intelligence Materials Science Division (2020 \sim)

1. Workshop for CALPHAD software and database

- FactSage annual Workshop (Feb. 23-25, 2022)
 - **201 online participants**: graduate students, researchers, and scientists
 - Organizer: Seoul National University (In-Ho Jung)
 - Two sessions: Pyrometallurgy applications & Alloy development



1. Workshop for CALPHAD software and database

- FactSage annual Workshop (Feb. 01-03, 2023)
 - **<u>120 onsite + 150 online participants</u>**: graduate students, researchers, and scientists
 - Organizer: Seoul National University (In-Ho Jung)
 - Two sessions: Pyrometallurgy applications & Alloy development



2. Workshops by KIMM Computational Materials Science division

1) KIMM Fall Meeting : 2023.10.26 (Thur)

- \cdot Subject : Future Semi-conduct Materials AI Computational Materials Science
- \cdot 11 Presentations and 100 participants

2) KIMM Fall Meeting – Tutorial session : 2023. 10. 25 (Wed)

- · Subject : Open database
- · 60 participants

3) Summer school of Computational Materials Science Division

- : 2023.06.28 (Wed)-30(Fri)
- · Subject : Molecular Dynamics
- · 73 participants

4) Summer school of Computational Materials Science Division

- : 2023.06.02(Fri)
- \cdot Subject : Multiscale modeling and Machine learning Potential
- · 89 participants

5) Winter school of Computational Materials Science Division

- : 2023.01.05(Thur) 06(Fri)
- \cdot Subject : Development of Catalyst : Current and Future
- · 89 participants



2. Workshops by KIMM Computational Materials Science division

6) Winter school of Computational Materials Science Division : 2023.01.09(Mon)-10(Tue)

- \cdot Subject : Development of Nuclear materials and fuels : Current and Future
- \cdot 57 participants
- 7) Tutorial session by Computational Materials Science Division : 2023.08.15(Wed)-17(Thur)
- \cdot Subject : ChatGPT and Materials development
- \cdot 184 participants
- 8) Special workshop : 2023.07.03(Mon) 05(Wed)
- \cdot Subject : Phase field model : Theory and Tutorial
- · 42 participants





2. Workshops by KIMM AI Materials Science

1) Winter School on artificial intelligence in MSE : Feb. 15-17, 2023

✓ Intermediate level training on artificial intelligence and related applications in MSE

✓ Over 60 Graduate students, Faculty, and Researchers from universities, research institutes, and companies

2) Summer School on artificial intelligence in MSE : Aug. 23-25, 2023

✓ Education for beginners in machine learning and deep learning

✓ Over 65 Graduate students, Faculty, and Researchers from universities, research institutes, and companies



3. Phase diagram activities (MEAM)

Ex.PD = Experimental phase diagram study	Contact person
Ex.TD = Experimental study of thermodynamic data	BJ. Lee (Postech): calphad@postech.ac.kr
CA = Critical Assessment of literature	WS. Ko (Ulsan Univ): wonsko@ulsan.ac.kr
TD Mod. = Thermodynamic Modeling, CALPHAD-type	J. Lee (Korea Univ): joonholee@korea.ac.kr
AS = Atomistic Simulations / First Principles	IH. Jung (Seoul National Univ): in-ho.jung@snu.ac.kr
Comment = notes on application etc., free text	Y.B Kang(Postech): ybkang@postech.ac.kr
F = finished during 2021	
X = work in progress	

System	Ex PD	Ex TD	CA	TD Mod.	AS	Comment	Contact person	Country
Na-Cu-Sn					F	2NN MEAM interatomic potential	BJ. Lee	KR
Na-Mn-Sn					F	2NN MEAM interatomic potential	BJ. Lee	KR
Na-Ni-Sn					F	2NN MEAM interatomic potential	BJ. Lee	KR
Mg-Mn					F	2NN MEAM interatomic potential	BJ. Lee	KR
Li-Ni-O					F	2NN MEAM interatomic potential	BJ. Lee	KR
Li-Ni-Mn-Co-O					F	2NN MEAM interatomic potential	BJ. Lee	KR
AI-O					F	2NN MEAM interatomic potential	BJ. Lee	KR
Nb-Sn					F	2NN MEAM interatomic potential	BJ. Lee	KR
Nb-Sn-Ti					F	2NN MEAM interatomic potential	BJ. Lee	KR
Au-Ti					F	2NN MEAM interatomic potential	WS Ko	KR
Pt-Ti					F	2NN MEAM interatomic potential	WS Ko	KR
Ni-Ti-Cu					F	2NN MEAM interatomic potential	WS Ko	KR
Cu-Al-Ni					X	2NN MEAM interatomic potential	WS Ko	KR
W-H					X	2NN MEAM interatomic potential	WS Ko	KR
Ni-Mo-W					X	2NN MEAM interatomic potential	WS Ko	KR
Fe-Cu-Sn					X	2NN MEAM interatomic potential	WS Ko	KR
Ti-Zr-Mn-Cr						ML (Hydrogen solubility in AB2 type alloys)	J. Lee	KR
Zr-Ti-Mn-V-Ni						ML (Hydrogen solubility in AB2 type alloys)	J. Lee	KR

3. Phase diagram activities (CALPHAD)

		1														
System	Ex PD	Ex TD	CA_	TD Mod.	AS Comment	Contact person	Country	System	Ex PD	Ex TD	CA	TD Mod.	AS	Comment	Contact person	Country
Fe-Sn	0		0	0	published		KR	Al-Co			0	0		completed	d d d d d d d d d	KR
Fe-As			0	0	completed	Y.B. Kang		Al-Ni			0	0		completed		
Fe-Sb			0	0	completed			Al-Ti			0	0		completed		
Fe-Pb			0	0	completed			Co-Cr			0	0		completed		
Sn-C			0	0	completed			Co-Mo			0	0		completed		
As-C			0	0	completed			Co-Ti			0	0		completed		
Sb-C			0	0	completed			Ni-Cr			0	0		completed		
Sn-S			0	о	published			Ni-Ti			0	0		completed		
Sb-S			0	О	published			Ni-Cr-Fe			0	0		completed		
Ag-S			0	о	published			Ni-Cr-Mo			0	0		completed		
Fe-Al-O			0	0	submitted			Ni-Fe-Mo			0	0		completed		
Fe-Ti-O	О		ο	о	submitted			Cr-Fe-Mo			0	о		completed		
Al-Ti-O	0		0	0	submitted			Ni-Cr-Ti			0	0		completed	IH. Junf	
Fe-Al-Ti-O	О		ο	о	submitted			Ni-Fe-Ti			0	о		completed	l	
Co-Cr-Fe-Mn-Ni-Ti			0	0	CALPHAD	BJ. Lee	KR	Ni-Mo-Ti			0	0		completed		
Co-Cr-Fe-Mn-Ni-Zr			ο	о	CALPHAD			Cr-Mo-Ti			0	о		completed		
								Cr-Fe-Ti			0	0		completed		
								Fe-Mo-Ti			0	0		completed		
								Ni-Cr-Co			0	0		completed		
								Ni-Fe-Co			0	0		completed		
								Ni-Mo-Co			0	0		completed		
								Co-Cr-Fe			0	0		completed		
								Fe-Mo-Co			0	0		completed		
								Ni-Ti-Co			0	0		completed		
								Ni-Co-Al			0	0		completed		

4. Representative projects: Government

Several projects related to:

(1) Materials Hub Projects (3~5 yr projects)
– Metallic system for light Metals (Al, Mg, Ti)

(2) Superalloy projects (3~5 yr projects)

- Ni super alloy and Co super alloy

(3) Nuclear : Molten Salt Reactor (~5 yr project)

- Salt database

4. Representative projects: Industry





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Steelmaking Consortium Project V (2023-2026): "Carbon Neutral Steelmaking Process" (13 industrial members)

- Sub-project A-i): H2-H2O addition in key oxide systems (P2O5-CaO-MgO-Al2O3-SiO2-FeO-Fe2O3) (1) H2 and H2O dissolution in slag, and (2) major solid hydroxide compounds and solutions in CaO-SiO2-H2O, CaO-P2O5-H2O, Al2O3-CaO-H2O, and Al2O3-SiO2-H2O up to high pressures

- Sub-project A-ii): P2O5 -containing systems for iron ore and DRI melting process P2O5-CaO-MgO-Al2O3-SiO2-FeO-Fe2O3-MnO-... system

- Sub-project A-iii): V and Nb oxide systems: CaO-MgO-Al2O3-SiO2-Na2O-FeOx-VOx system and CaO-MgO-Al2O3-SiO2-Na2O-FeOx-NbOx system

- Sub-project A-iv): Expansion of Rare earth (RE) oxide containing systems: CaO-MgO-Al2O3-SiO2-FeO-Fe2O3-RE2O3 system

Sub-project A-v): Other minor oxide systems. (a) Hydroxides phases like hydrogarnets, hydrotalcite (solid solution at low temperature) for leaching of slag (Cr and V leaching), (b) V, Cr and Ti solubility (about a couple of percents) in Ca2(Al, Fe)2O5 for BOF slag, (c) solubility of V in C2S-C3P solid solution, (d) solubility of Cr oxide in mullite solid solution, (e) CaO-SiO2-ZrO2-Y2O3 system for Y2O3 stabilized ZrO2 in continuous casting environment.

- Sub-project A-vi): Tramp elements in liquid and solid steel: Sn, P, Cu, Zn, Ni, Cr, Mo, Pb, Cd, As in Steel database - additional project: MgO solubility in CaO-Al2O3-SiO2-FeO-Fe2O3 slag system