Report to 2021 APDIC

Activities in 2021 Korean Committee of Computational Materials Science and Engineering

May 15, 2022

In-Ho Jung

1. Thermodynamic Calculation Training

- **FactSage annual Workshop (Feb. 03-05, 2021; Virtual workshop)**
  - Over 120 graduate students and researchers from companies
  - Organizer: Seoul National University (In-Ho Jung)
  - Pyrometallurgy applications & Alloy development
  - Self learning videos available : http://in-ho-group.snu.ac.kr/?page_id=438
- **FactSage special workshop for MOLTEN 2021 conference (Feb. 15~19, 2021; Virtual workshop): Pyrometallurgical application**
  - Over 80 graduate students and researchers from companies
  - Organizer: Seoul National University (In-Ho Jung)

2. Workshops for Artificial Intelligence in Materials Science

- **Artificial Intelligence in Materials Science: New division (committee) in Korean Institute of Metals and Materials (KIMM)**
  - Foundation: Feb. 2020
  - Aims:

    (1) Promote the AI and Machine Learning methodology to materials science and engineering community.

    (2) Develop discussing groups for AI and ML in KIMM.
  - Activities:
    - <u>Organize 5 workshops in 2020 and 2021 (2~3days; beginner and intermediate level) for AI and ML in materials science – total registration: about 500 attendee.</u>
    - Organize special symposiums in KIMM spring and fall meetings

3. Phase diagram activities (MEAM)

Ex.PD = Experimental phase diagram study	Contact person
Ex.TD = Experimental study of thermodynamic data	B.-J. Lee (Postech): calphad@postech.ac.kr
CA = Critical Assessment of literature	W.-S. 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	I.-H. 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	

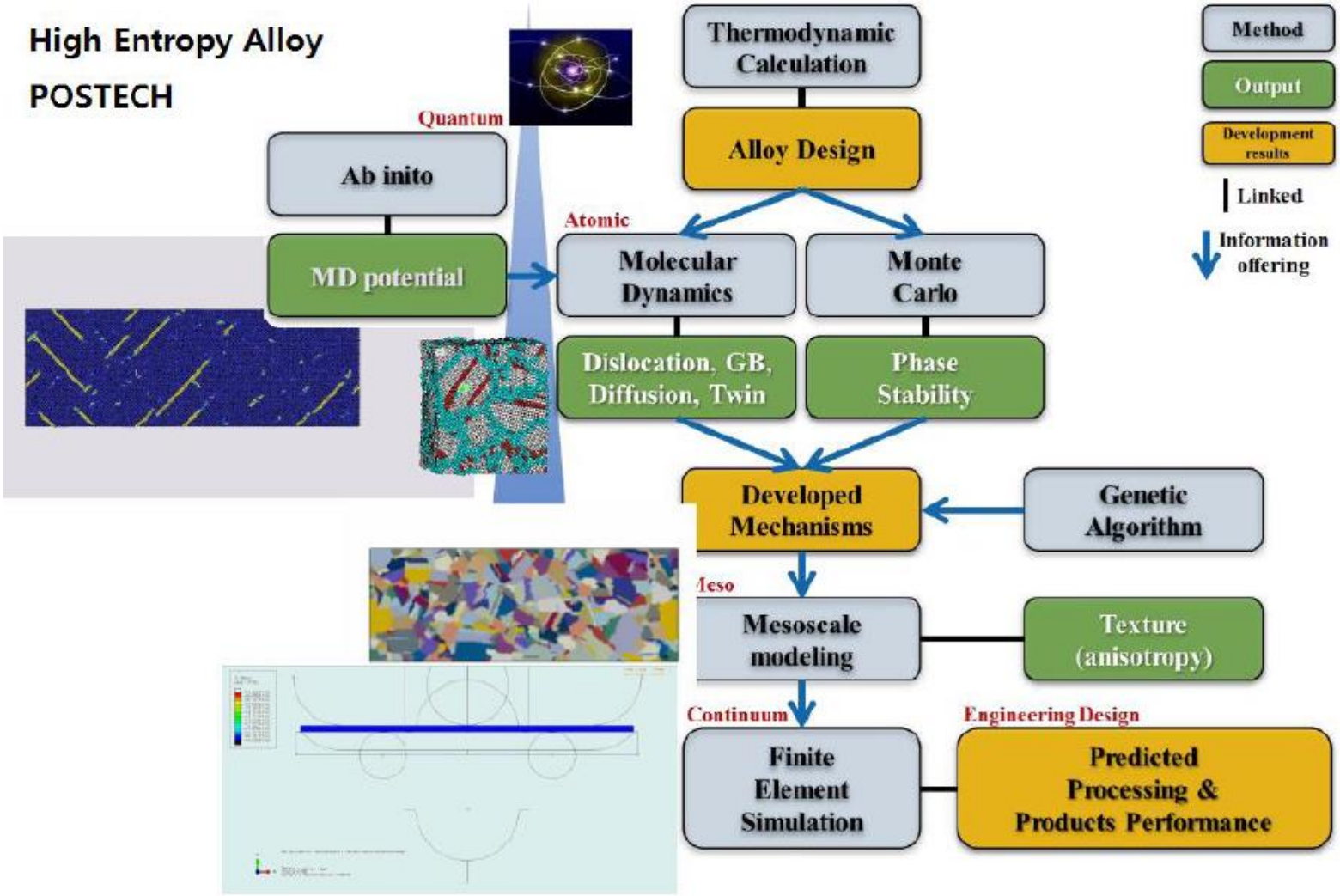
System	Ex PD	Ex TD	CA	TD Mod.	AS	Comment	Contact person	Country
Ag-Cu-Sn					F	2NN MEAM interatomic potential	W.-S Ko	KR
Nb-Ni-Ti					F	2NN MEAM interatomic potential	W.-S Ko	KR
Cu-Al-Ni					X	2NN MEAM interatomic potential	W.-S Ko	KR
Au-Ti					X	2NN MEAM interatomic potential	W.-S Ko	KR
Pt-Ti					X	2NN MEAM interatomic potential	W.-S Ko	KR
Na-Sn-Cu					F	2NN MEAM Interatomic Potential	Lee, B.-J.	KR
Na-Sn-Mn					F	2NN MEAM Interatomic Potential	Lee, B.-J.	KR
Na-Sn-Ni					F	2NN MEAM Interatomic Potential	Lee, B.-J.	KR
Nb-Sn					F	2NN MEAM Interatomic Potential	Lee, B.-J.	KR
Nb-Sn-Ti					F	2NN MEAM Interatomic Potential	Lee, B.-J.	KR
Li-Ni-O					F	2NN MEAM Interatomic Potential	Lee, B.-J.	KR

3. Phase diagram activities (CALPHAD)

System	Ex PD	Ex TD	CA	TD Md	AS	Comment	Contact person	Country
Fe-Sn	X		X	X			Y.-B. Kang	KR
Fe-Sn-C	X	X	X	X			Y.-B. Kang	KR
Fe-As-C	X	X	X				Y.-B. Kang	KR
Fe-Pb-C	X	X	X				Y.-B. Kang	KR
Fe-Sb-C	X	X	X				Y.-B. Kang	KR
Al-Ti-O	X		X	X			Y.-B. Kang	KR
Fe-P	F		F	F			Y.-B. Kang	KR
Fe-C-P	F		F	F			Y.-B. Kang	KR
Na-Zr-O	X		F	F			I.-H. Jung	KR
Sn-O	X		F	F			I.-H. Jung	KR
Sn-Si-O	X		F	F			I.-H. Jung	KR
Sn-Ca-O	X		F	F			I.-H. Jung	KR
Sn-Fe-O	X		F	F			I.-H. Jung	KR
Sn-Mg-O	X		F	F			I.-H. Jung	KR
Sn-Al-O	X		F	F			I.-H. Jung	KR
Sn-Zn-Si-O	S		F	F			I.-H. Jung	KR
Sn-Ti-Zr-O	X		F	F			I.-H. Jung	KR
Si-C-N			F	F			I.-H. Jung	KR
Ni-RE (rare earth)			F	F		16 binaries	I.-H. Jung	KR
Cr-RE (rare earth)			F	F		16 binaries	I.-H. Jung	KR
Co-RE (rare earth)			F	F		16 binaries	I.-H. Jung	KR
Co-Cr-Fe-Mn-Ni			F	F	F		Lee, B.-J.	KR
Bi-Sn				F	Effect of Pressure		J. Lee	KR
Ga-In				F	Effect of Pressure		J. Lee	KR
SFCA	X		Silico-ferrite of calcium and aluminum containing ZnO				J. Lee	KR
Bi-Sn				X	Nano Phase Diagram		J. Lee	KR

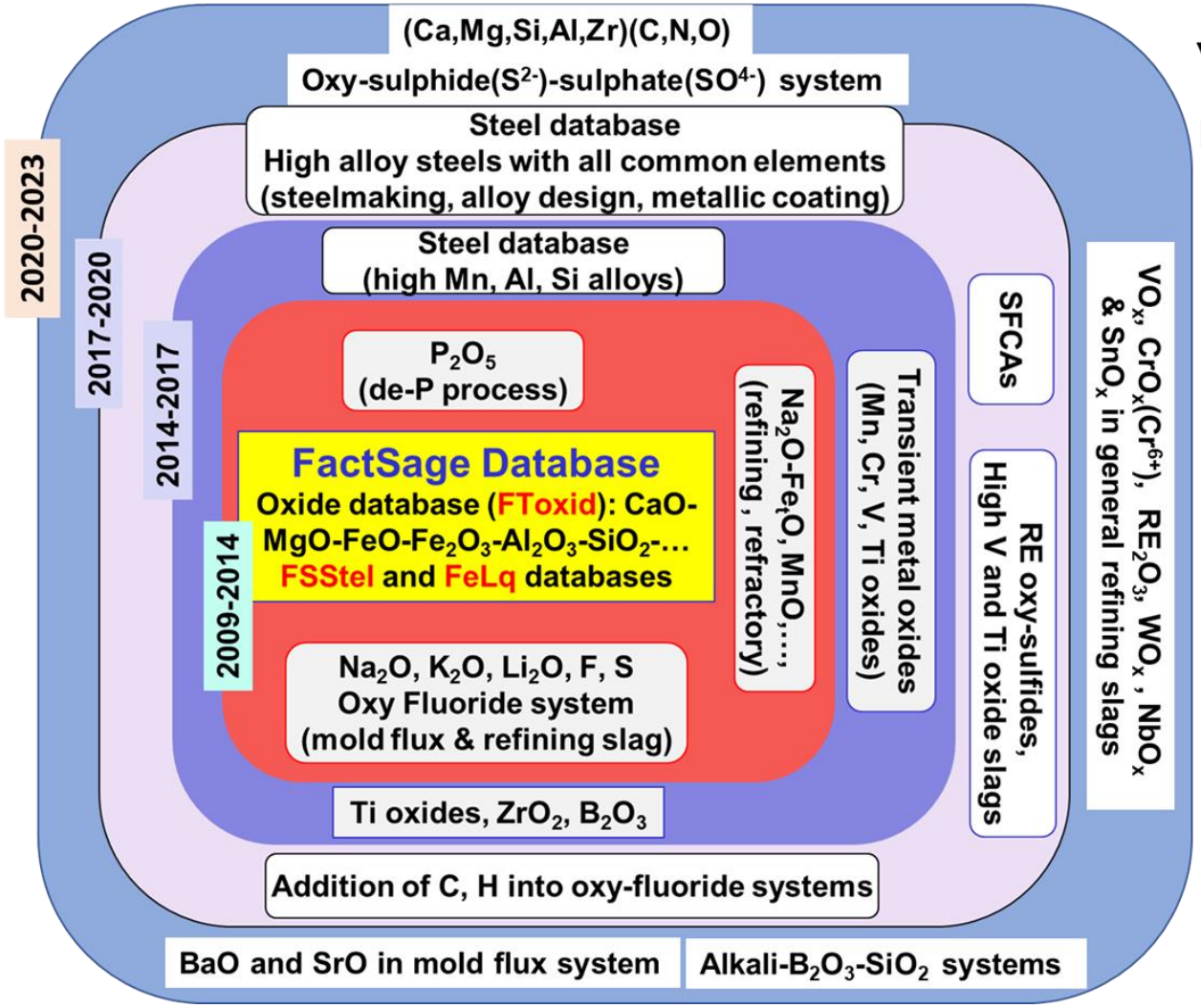
4. Representative projects: Government

(2016 – 2022)



4. Representative projects: Industry

Steelmaking consortium Project: In-Ho Jung (Seoul National University)



5. Publications

1. “Atomistic simulations of the deformation behavior of an Nb nanowire embedded in a NiTi shape memory alloy”, Jung Soo Lee, Won-Seok Ko, B. Grabowski,, Acta Materialia 228, 117764 (2022).
2. “Atomistic simulations of Ag-Cu-Sn alloys based on a new modified embedded-atom method interatomic potential”, Won-Seok Ko, Jung Soo Lee, Dong-Hyun Kim, Journal of Materials Research 37, 145-161 (2022).
3. "Uniqueness of a Correction to Interaction Parameter Formalism in a Thermodynamically Consistent Manner", Youn-Bae Kang, Metall. Mater. Trans. B, 51B(2020) 795.
4. "Critical Evaluation and Thermodynamic Modeling of the Fe–P and Fe–C–P system", Michael Bernhard, Youn-Bae Kang, Peter Presoly, Aimen E Gheribi, and Christian Bernhard, Calphad, 70(2020), 101795.
5. "Experimental Study of High Temperature Phase Equilibria in the Iron-Rich Part of the Fe-P and Fe-C-P Systems", Michael Bernhard, Peter Presoly, Nora Fucks, Christian Bernhard, and Youn-Bae Kang, Metall. Mater. Trans. A, 51(2020), 5351.
6. "Thermodynamic Modeling of Liquid Steel", Youn-Bae Kang, ISIJ Int., 60(2020), 2717.
7. "Phase Equilibria of Al2O3–TiOx System under Various Oxygen Partial Pressure: Emphasis on Stability of Al2TiO5–Ti3O5 Pseudobrookite Solid Solution", Young-Joon Park, Wan-Yi Kim, and Youn-Bae Kang, J. Euro. Ceram. Soc., 41(2021), 7362.
8. "Progress of Thermodynamic Modeling for Sulfide Dissolution in Molten Oxide Slags: Sulfide Capacity and Phase Diagram", Youn-Bae Kang, Metall. Mater. Trans. B, 52(2021), 2859
9. “Pressure dependence of thermodynamic interaction parameters for binary solid solution phases: an atomistic simulation study,” Sang-Ho Oh, Xiao-Gang Lu, Qing Chen, Byeong-Joo Lee, CALPHAD 75, 102342 (2021).
10. “Computational design of V-CoCrFeMnNi high-entropy alloys: An Atomistic Simulation Study,” Won-Mi Choi, Jin-Soo Kim, Won-Seok Ko, Dong Geun Kim, Yong Hee Jo, Seok Su Sohn, Sunghak Lee, Byeong-Joo Lee, CALPHAD 74, 102317 (2021).
11. “Alloying non-precious metals into Ni-based electrocatalysts for enhanced hydrogen oxidation reaction in alkaline media: A computational study,” Jin-Soo Kim, Jeong Woo Han and Byeong-Joo Lee, Applied Surface Science 554, 149627 (2021).
12. “Second nearest-neighbor modified embedded-atom method interatomic potentials for the Mo-M (M = Al, Co, Cr, Fe, Ni, Ti) binary alloy systems,”
    Sang-Ho Oh, Jin-Soo Kim, Chang Seo Park and Byeong-Joo Lee, Compu. Mater. Sci. 194, 110473 (2021).
13. “The origin of activation of non-basal slip in Mg-Ce dilute alloy - An atomistic simulation study,”
    Jong-Kwan Lee and Byeong-Joo Lee, Met. Mater. Trans. A, 52A, 964-974 (2021).
14. “Second-nearest-neighbor modified embedded-atom method interatomic potential for V-M (M = Cu, Mo, Ti) binary systems,” Jaemin Wang and Byeong-Joo Lee, Compu. Mater. Sci. 188, 110177 (2021).
15. “Modified embedded-atom method interatomic potentials for Mg-Al-Ca and Mg-Al-Zn ternary systems,”
    Hyo-Sun Jang, Donghyuk Seol and Byeong-Joo Lee, J. Magnesium and Alloys 9, 317-335 (2021).

5. Publications

16. Huije Ryu, Yangjin Lee, Hyun Jung Kim, Seoung Hun Kang, Yoongu Kang, Kangwon Kim, Jungcheol Kim, Blanka E. Janicek, Kenji Watanabe, Takashi Taniguchi, Pinshane Y. Huang, Hyeonsik Cheong, In Ho Jung, Kwanpyo Kim, Young Woo Son, Gwan Hyoung Lee, “Anomalous Dimensionality-Driven Phase Transition of MoTe2 in Van der Waals Heterostructure”, Advanced Functional Materials, 2021, 31(51):2107376.
17. Jaesung Lee, Sunyong Kwon, and In-Ho Jung, “Phase Diagram Study and Thermodynamic Assessment of the Na_2O-ZrO_2 System”, J. Euro. Ceram. Soc, 2021, Vol. 41, pp. 7946-7956
18. Jian Wang, Dong Han, Zhang Zhang, In-Ho Jung, and Wei-feng Rao, “Experimental measurement and thermodynamic evaluation of the Mg + Cu + Sr ternary system”, J. Chem. Thermodynamics, 2021, 163, 106582.
19. Tiantian Yin, Jaesung Lee, Elmira Moosavi, In-Ho Jung, “Critical Evaluation and the Thermodynamic Optimization of the Sn-O System”, Ceramics International, 2021, Vol. 47 (20), pp. 29267-29276.
20. Jian Wang, Zhang Zhang, In-Ho Jung, Wei-Feng Rao, “Critical evaluation and thermodynamic optimization of the Ag-X (X=Mn, Y, Sr) binary systems” Intermetallics, Vol. 136, 2021, 107260.
21. Jian Wang, Zhang Zhang, In-Ho Jung, Liyuan Sheng, “Experimental investigation and thermodynamic modeling of the Mg–Sn–Sr ternary system”, Calphad, 2021, Vol. 72, 102237.
22. Jimmy Rojas, In-Ho Jung, Arun Majumdar, "Computational Discovery of Metal Oxides for Chemical Looping Hydrogen Production" Cell Reports Physical Science, 2021, Volume 2, Issue 3, 100362.
23. Ho-Gil Choi, Seungwoo Choi, Min-Kyung Kim, Juyoung Jang, Ki Tae Nam, In-Ho Jung, Kyung-Woo Yi (2021) Electrolysis of iron with oxygen gas evolution from molten sodium borate electrolytes, Ironmaking & Steelmaking, DOI: 10.1080/03019233.2020.1861837
24. Sun Yong Kwon, Reghan J. Hill, In-Ho Jung, “A model for multicomponent diffusion in oxide melts”, Calphad, 2021, vol. 72, 102246.
25. Sourav Panda and In-Ho Jung, “Coupled Experimental Study and Thermodynamic Modeling of the Fe–Mn–Ti–O System”, Metals and Materials Inter., 2021, volume 27, pp. 725–743.
26. Arijit Biswas, Chandan Sahoo, Wei-Tong Du, In-Ho Jung, and Manas Paliwal, “New production route for Vanadium Nitride master alloy : Experimental and thermodynamic analysis”, Metall. Mater. Trans. B, 2021, 52, pp. 956–967.
27. Zhimin You and In-Ho Jung, “ Thermodynamic optimization of the Mn–P and Fe–Mn–P systems”, Calphad, 2021, vol. 72, 102226.