

CALPHAD 2024 Poster Presentations

Title	Name
Towards modelling the PBF-LB process of a MgZnCa alloy	Alonso Rancurel, Belén
Ocean of Data: Tools for Data Generation of Single Phases	Amaral, Ricardo
Experimental phase equilibria study and thermodynamic modelling of the CaO-MgO-FeO-Fe ₂ O ₃ -SiO ₂ system	Babaian, Igor
High-pressure phase diagram of Bi-Ga: Polymorphism, anomalous melting curves and liquid miscibility gap	Ben Shalom, Shir
From raster data to insights: Statistical microstructure characterization through composition and local property fields	Benito, Santiago
Thermodynamic modelling of chlorides systems for Molten Salt Reactor Application	Chatain, Sylvie
First-principles and machine learning prediction of stability and structural properties of transition metal HEAs	Chen, Ying
Mean-field model for hydride evolution within Zircaloys	Cladingboel, Connor
Diffusion and Thermodynamic Modeling of the Effects of Substrate Aluminum Content on Coating-Substrate Interactions During Resistance Spot Welding of Galvanized 3rd Generation Advanced High Strength Steels	Colburn, Jake
Approaches to model the growth of nickel oxide on nickel	Craven, Harry
Ordering regimes in zirconium carbide	Davey, Tessa
Development of thermodynamic database for Li recycling	de Abreu, Danilo Alencar
Phase equilibria and solubility limits in the (Ce-Nd)-Fe-B system for new substituted permanent magnets	de Villoutreys, Eloi
A data-driven study of the enthalpy of mixing in the liquid phase	Deffrennes, Guillaume
HP-HT modelling of Fe-Mg system: A comparison of CALPHAD-compatible models and data acquisition.	Desseaux, Mathias
High Throughput Calculation at Steel Phase Diagram with Calphad and Bayesian Artificial Neural Network	Dinçer, Mehmet Şamil
Sampling-free thermodynamics in bulk crystalline metals from the mean-field anharmonic bond model	Dsouza, Raynol
Thermodynamic modeling of the CaO-CaF ₂ -B ₂ O ₃ -BF ₃ reciprocal system	Ed-Dahri, Soukaina
Thermodynamic modelling of the ZrO ₂ -Ta ₂ O ₅ and Y ₂ O ₃ -Ta ₂ O ₅ systems	Fabrichnaya, Olga
Phase equilibria, microsegregations and mechanical properties of Inconel 718 alloy samples processed in electromagnetic levitation facility	Fang, Yindong
Poster: Thermodynamic database for the FeCrMoNiN system	Frisk, Karin
Automated Calphad Optimization Workflow	Frueh, Cassie
Modeling of solidification microstructures with non-equilibrium effects at interfaces with Calphad data	Gandin, Charles-André
Thermodynamic assessment of the Al ₂ O ₃ -Fe ₂ O ₃ -FeO system by introducing the AlO ₂ -1 species into the thermodynamic model for liquid phase	Gao, Fengyang
High-temperature refractory Al-M-Si-O (M= Nb, Ta) systems	Gebauer, Julian
Ocean of Data: AI-driven High-throughput CALPHAD Modeling	Gong, Rushi
Estimating the Yield Strength of Ni-based Superalloys with CALPHAD and KWN for Varying Aging Conditions	Govercin, Betul
Phase-field simulation of core-rim structure at the early sintering stage in TiC-WC-Ni cermet	Guan, Yiqi
Experimental investigation and thermodynamic description of the Co-Mo-Ta system	Guo, Cuiping
Study on the $\gamma + \gamma'$ microstructure characterization of the Co-V-Zr system based on CALPHAD method	Guo, Cuiping
Carbon solubility in solvent for SiC rapid solution growth: Thermodynamic evaluation of Si-Cr-Ce-C system	Guo, Zhongnan
Phase Equilibrium Investigations of the HfO ₂ -Y ₂ O ₃ -Ta ₂ O ₅ System	Habermann, Alina
Using the Calphad Optimizer (CO) for the assessment of the Gibbs energies of non-stoichiometric Perovskites in the system Ca-Mn-Sr-O	Hack, Klaus
The structural, energetic and dehydrogenation properties of pure and Ti-doped Mg(0001)/MgH ₂ (110) interfaces	Han, Bo
Thermal stress analysis of WC-Co-Ni hard alloys based on thermodynamic calculations	He, Meiling
Modeling Multi-Phase Precipitation Kinetics in Al-Mg-Si alloys including Metastable-Stable Phase Transitions	Hwang, Da Weon
The K ₂ O-SiO ₂ -CO ₂ system	Ilatovskaia, Mariia
CALPHAD-informed phase-field modeling of incipient melting in oxidized fuel: U-Pu-O, a new step toward multicomponent systems	Introïni, Clément
From ab initio calculations to alloy phase diagrams: automated workflows with pyiron	Janssen, Jan
Phase equilibrium of the Fe ₂ O ₃ -TiO ₂ system	Jiao, Mengjiao
Experimental and computational study on phase diagram thermodynamics of the Cu-Cr-Zr-Mg-Y system	Jing, Fengting
Hybrid data-driven thermodynamically-based temperature modeling of secondary steelmaking	Kavić, Daniel
Ocean of Data: Efficient Data Infrastructure for Materials	Krajewski, Adam
Thermodynamic Modeling of the Cu-Sn system: Considering the crystallography of NiAs/Ni ₂ In-type phases	Kriegel, Mario J.

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CALPHAD-based ICME Design for Crack-free Wire-Arc Additive Manufacturing of Functionally Graded Alloy from Copper Alloy C18150 to Superalloy Inconel 625	Ladinos-Pizano, Luis
A Third Generation CALPHAD Description of Pure Nb	Larsson, Felicia
CALPHAD-based Prediction of Evaporation in Multi-component Melt Pool during Additive Manufacturing Process	Lee, Matae
Modelling the transport of hydrogen around melt-pools formed by moving heat sources.	Leeman, Jack
Experimental investigation and thermodynamic evaluation of the ZrO ₂ -TiO ₂ -SrO system	Li, Chonghe
Experimental investigation and computational thermodynamics of the quaternary system Fe-C-Mn-S	Littringer, Robert
Building high-dimensional phase diagram with machine learning (ML) accelerating and the cost lowering by phase space analysis	Liu, Zhengdi
Preliminary results on the experimental investigation of the liquidus projection of the Al-Ti-Hf ternary system	Luiz, Jéssica
Experimental investigation and thermodynamic description of selenium-based systems	Mikšík, Dávid
Extending universal interatomic potential for grain boundary segregation in steel	Mohandas, Naveen Karuthodi
Thermo-Kinetics of Impurities in Uranium Alloys	Moore, Emily
Thermodynamics of the Na ⁺ , K ⁺ , Mg ²⁺ , Ca ²⁺ // Cl ⁻ , SO ₄ ²⁻ multi-component system for the identification of potential salt-based high temperature Phase Change Materials	Morsa, Amedeo
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Recent developments in the TCS Mg-based alloys database	Noori, Mehdi
Gas phase from K ₂ TaF ₇	Nuta, Ioana
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Parameterization of a CALPHAD-informed phase-field model to simulate incipient melting in oxidized fuel	Plumecocq, Clément
Defect Phase Diagrams at Ab-Initio Accuracy with Machine Learning Potentials	Poul, Marvin
Using automated thermodynamic simulations for the development of new Cu alloys with high strength and good electric conductivity	Preußner, Johannes
Thermodynamic assessment of the fcc/hcp transformation in Fe-Mn alloys	Rackwitz, Julian
Thermodynamic assessment of Si-Zr and Cu-Si-Zr systems	Rajkumar, V. B.
Thermodynamic assessment of Cr-Mo-Si system	Ramasamy Chitra, Arun
Modeling of kinetics of phase/pore formations in compositionally graded Ni-based superalloys under isothermal conditions: A CALPHAD-Phase field study	Riyahi khorasgani, Ahmadreza
Triplex steels in-situ grain refinement in Laser-Powder Bed Fusion	Sanchez-Poncela, Manuel
Optimized Synthesis of Reactive MgO from Rejected Brine via Integrated Thermodynamic Solution Modelling and Experimental Parameter Study	Senevirathna, Hasanthi L.
Experimental Investigation of the Mg-Sn-Gd Alloy System Assisted by First-Principles Calculations	Shandley, Rohit
Current results on the investigation of kinetic parameters of VAl ₃ , V ₅ Al ₈ and (V)	Silveira, Vitória
Thermodynamic description of concentration and diffusion of point defects in metals and compounds	Starikov, Sergei
A proposal for an XML based format for Calphad databases	Sundman, Bo
Effect of strain energy on the formation of G.P. zone in the Al-Cu binary system	Suzuki, Takao
Thermodynamic Modeling of Sodium Salt Solubility in Black Liquor	Talebi, Sina
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Metastable defect phase diagrams as roadmap to tailor chemically driven defect formation	Tehranchi, Ali
Data-centric detection of compounds containing wrong data in large Calphad databases	to Baben, Moritz
Towards the improvement of liquid Gibbs energy assessment by the assimilation of surface tension data	Tourneix, Arthur
Integrated Computational Materials Engineering (ICME) to Develop Electrical Contacts for Thermoelectric Devices	Tumminello, Silvana
Kawin: An open source tool for Calphad-based kinetics	Ury, Nick
Screening of alloying elements and their combinations to improve the corrosion resistance of Mg alloys through high throughput calculations	Wang, Jun
CALTPP: an intelligent software to evaluate thermophysical properties	Wen, Shiyi
NIST data resource for curated thermophysical property data of metal systems	Wilthan, Boris
High-throughput determination of interdiffusivities for quaternary system: a case study on Ni-Co-Al-Ta system adopting triple and quadruple techniques	Wu, Xue-Ting
Simulation of solidification paths and phase formation in the Mg-rich corner of Mg-Ca-Zn alloys	Xie, Yanheng
Suitability of slag solution models as the basis for thermophysical properties - A review	Zaيمان, Stéfan

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High-throughput determination of the interdiffusion coefficients and atomic mobilities in bcc Ti-Fe-V alloys	Zhang, Hongyu
Phase equilibria in the FeO-Fe ₂ O ₃ -X (X = SiO ₂ , MgO) systems: Experimental measurement and thermodynamic modeling	Zhang, Liang
Simple Yet Robust Models of Diffusion Coefficients for CALPHAD Mobility Databases	Zhao, Ji-Cheng
A computationally highly efficient ab initio approach for melting property calculations and practical applications	Zhu, Lifang
Measurement of Thermal Conductivity and Thermal Diffusivity Through Spatial and Temporal Temperature Gradients in a Single Device	Zhuo, Junsheng