Poster presentations

Monday, June 12, 2017, 15:30-18:00
Poster session A, chair: M. Perrut

PA1 Thermodynamic modeling of long-term precipitation kinetics in heat-resistant alloys, **Shim Jae-Hyeok**

PA2 Analysis of the phase equilibria and phase transformations in the region Al-Al_3Zr during slow cooling rate solidification and long-time annealings below the solidus, **Khvan Alexandra**

PA3 Thermodynamic Optimization of Ni-Ti-V Ternary System, **Kathirvelu Santhy**

PA4 Computational Study of Atomic Mobility in HCP Mg-Al-Zn Ternary Alloys, **Wang Jingya**

PA5 High-throughput Investigation of Diffusion and creep Micro-Mechanical Properties in Mg alloys, **Li Na**

PA6 A study of the Mg-Al-C system: synthesis and thermal stability of the Al_2MgC_2 ternary carbide, **Deffrennes Guillaume**

PA7 Integration of Phase Equilibrium Calculation and Kinetic Simulation, **Chen Shuanglin**

PA8 Influence of W and Mo on the phase equilibrium and diffusion behaviour of Ni-Co-Al ternary system, **Wang Yang**

PA9 Aqueous Salt Hydrates: Unconventional Deep Eutectic Solvents, **Marcus Yizhak**

PA10 High pressure-high temperature phase diagram using electrical resistance measurements in a Paris-Edinburgh large volume press, **Emuna Moran**

PA11 Ab initio study of the phononic origin of negative thermal expansion, **Argaman Uri**

PA12 Al-B-C ternary compounds : synthesis, structure, composition and thermal stability, **Dezellus Olivier**

PA13 Comparison of various DTA methods for liquidus determination in Ag-Cd-In alloys, **Gajavalli Sai**

PA14 Thermodynamic modelling of the Al-Co-Pd system, aluminium rich corner of the phase diagram, **Homolova Viera**

PA15 Thermodynamic modelling of Fe-Cr-Ni and its implication for the calculation of multicomponent systems, **Jacob Aurélie**

PA16 Influencing factors of atomic order in binary sigma phases, **Liu Wei**

PA17 First-principles Calculation Assisted Thermodynamic Modeling of B-Ta and B-C-Ta System, **Xuemei Ouyang**

PA18 Experimental Investigation and Thermodynamic Calculation of Phase Equilibria in the Sn-Zn-Co Ternary System, **Hu Jingxian**

PA19 Phase equilibria, Thermodynamic Assessments and Microstructure Development of Mg-Alkaline Earth-Rare Earth Systems, **Xu Guanglong**

PA20 Investigation of the ternary Ag-Ga-Sn phase diagram, **Premovic Milena**

PA21 Experimental investigation and phase equilibria of Al-Zn-Cu system, **Zhang Yuhui**

PA22 Experimental investigation and thermodynamic modeling of Co-Ge system, **Zeng Yinping**

PA23 A thermodynamic study of the WC-(Fe,Co,Ni) hardmetal, **Peng Zhou**

PA24 Phase Equilibria and Thermodynamic Modelling in the System Ni-Sn-Zr, **Vrestál Jan**

PA25 Phase equilibria of Sn-Ag-In-Zn quaternary system, **Chen Sinn-Wen**

PA26 Thermodynamic and TEM investigations of Si poisoning effects on grain refinement in Al-Ti-Si and Al-Nb-Si systems, **Li Yang**

PA27 Isothermal sections of Mg-La-Zr system in Mg-rich corner at 300, 400 and 500° C, **Zhu Wenfei**

PA28 Phase Equilibria of 540° C Isothermal Section of Fe-Al-Zn-Ce System, **Zhi Li**

PA29 Phase stability of ternary compounds in Cu-Li-Sn system and path hysteresis in Cu_6Sn_5 electrode, **Jianchuan Wang**

PA30 Thermochemistry of some Bismuth-Transition metal compounds by high temperature direct synthesis calorimetry, **Meschel Susan V.**

PA31 Modelling solidification segregation in two Nb microalloyed steels, **Costa E Silva Andre**

PA32 Experimental study of Al-Cu-Zn phase diagram, **Zobac Ondrej**

PA33 Thermodynamic investigations of Fe-Mn-Al-Ni shape memory alloys, **Walnsch Alexander**

PA34 Optimization of compositions and physical properties of salt systems for latent heat storage in thermal solar energy applications, **Gheribi Aimen Ernest**

PA35 Ternary diffusivity from both the intersection of two diffusion couple and single diffusion couple: application to the Cu-Ni-Sn ternary system, **Du Changfa**

PA36 The stability investigation of $Fe_{23}Zr_6$ in the Fe-Zr system, **Zou Nan**

PA37 First principles study of hydrogen diffusion in iron, **Hirata Kenji**

PA38 Thermodynamic evaluations of the local ordering behaviors in the LPSO-forming Mg-Zn-Y system, **Egami Mariko**

PA39 Thermodynamic re-assessment of the Al-Fe-Mn system, **Zheng Weisen**

PA40 Study of thermal stability of doped CoSb based skutterudites by Knudsen effusion mass spectrometry, **Zelenka Frantisek**

PA41 Study of thermal stability of $CoSb_3$ skutterudite by Knudsen effusion mass spectrometry, **Broz Pavel**

PA42 Contribution to the experimental determination of the Ti-Al-W phase diagram, **Vaubois Thomas**

PA43 Mixing enthalpy measurements of liquid Li-Pb-Sb alloys, **Terlicka Sylwia**

PA44 Phase equilibria, thermodynamics and microstructure simulation of metastable spinodal decomposition in metastable c-TiAlN-based coatings, **Zhou Jingjing**

PA45 Cluster ordering of Mg-LPSO, **Nishitani Shigeto**

PA46 Thermodynamic descriptions of the quaternary Al-Si-Mg-RE (RE=Sc, Ce) systems and their application to design RE-containing cast aluminium alloys, **Lu Zhao**

PA47 Experimental Investigation of the Fe-Co-Ce System, **Fartushna Iuliia**

PA48 Experimental investigation and thermodynamic re-assessment of the ZrO_2-TiO_2 system, **Saenko Ivan**

PA49 Stability and defect chemistry analysis of Cu-doped Ceria by computational thermodynamic modelling, **Mcinnes Gregor**

PA50 Phase equilibria of binary Cr-Os system: experimental measurement and thermodynamic assessment, **Lin Yan**

PA51 Modeling of the Mn-Ni-Pd alloy system, **Brosh Eli**

PA52 Thermodynamic modelling of the B - Mn - V system, **Kepic Jan**

PA53 Experimental and computational study of diffusion between Fe-Cr-Al and Fe-Ni alloys at 800° C and 1000°, **Ojha Rohit**

PA54 On the configurational entropy of nano-solutions, **Kaptay George**

PA55 Thermodynamic Modelling of the Al-Mn-C System, **Tang Florian**

PA56 Phase equilibria of the Gd-Mn-Ge/Si ternary systems and magnetic properties of $GdMn2(Ge,Si)_2$ compound, **Wang Jiang**

PA57 Experimental study and thermodynamic calculation of Mn-RE (RE=Nd, Gd, Ho, Dy) binary systems, **Wang Jiang**

PA58 Development of a new thermodynamic database for slag relevant oxide systems containing P_2O_5, **Yazhenskikh Elena**

PA59 Electronic state entropy: informing thermodynamic and transport properties of the molten state., **Allanore Antoine**

PA60 Solidus surface projection of Fe-Sn-S system, **Sinyova Svetlana**

PA61 Phase Equilibria of the Fe-Al-Zr System at 600°C, **Zhao Manxiu**

Tuesday, June 13, 2017, 15:30-18:00
Poster session B, chair: M. Perrut

PB1 Experimental study on Fe-C-La system, **Mardani Masuma**

PB2 Wetting and interfacial reactivity in the Al_3Ti-SiC system, **Gambaro Sofia**

PB3 Experimental study of phase equilibria of the La/Y-Fe-B ternary systems, **Wang Jiang**

PB4 Thermodynamic optimization of Al-B-N system using ab initio calculations, **Sridar Soumya**

PB5 Prediction of heat capacity, **Zienert Tilo**

PB6 Thermodynamic study and assessment of the fluorine-iron system, **Chatain Sylvie**

PB7 Effects of Ni-doping on various properties of NbH phases: A First-principles investigation, **Wang Zhongmin**

PB8 Effects of Mo alloying on the structure and hydrogen-permeation properties of Nb metal, **Wang Zhongmin**

PB9 Evaluation of empirical rules on the phase formation of the multi-principal element alloys through Calphad approach, **Liang Song-Mao**

PB10 Ab initio calculations of the intermetallics in Ni-Zr system, **Jana Asmita**

PB11 Thermodynamic modeling of the Co-Cr-Ta system, **Yao Wang**

PB12 Experimental research on thermo-stability of the ternary compounds and related phase transformation in the Mg-Zn-Gd system, **Li Hong-Xiao**

PB13 Remodelling of Hf-V system, **Pavlu Jana**

PB14 Thermodynamic Evaluation and Optimization of the NaF - KF - ZnF_2 System, **Aubé Maxime**

PB15 Thermodynamic modelling of key metallic sub-systems for the treatment of mid-level wastes, **Soldi Luca**

PB16 Thermodynamic description of the Ga-Li-Zn system, **Dębski Adam**

PB17 The characteristic of Fe as a β-Ti stabilizer in Ti alloys, **Guo Yanhua**

PB18 Structure, elasticity and thermal decomposition of $Ti_{1-x}TM_xN$ alloys from first-principles study, **Jiong Wang**

PB19 Calculation of mixing enthalpy in Mo-Pd-Rh-Ru system, **Crivello Jean-Claude**

PB20 Experimental and computational study on surface layer microstructure evolution in single crystal superalloys during solution heat treatment, **Spathara Dimitra**

PB21 Experimental Determination of Phase Equilibria Related to Iron Silicides in the Fe-Si Binary System, **Han Kwangsik**

PB22 Theoretical study of hydrogen insertion in bcc metals, **Bourgeois Natacha**

PB23 Experimental investigation and thermodynamic calculation of the Al-Si-V system in the Al-rich corner, **Li Kang**

PB24 CALPHAD assessment of the key ternary and quaternary systems in Ti alloys, **Hu Biao**

PB25 Liquidus and solidus projections of the Fe-Co-S system, **Ilatovskaia Mariia**

PB26 Phase Equilibria of the Gd-Fe-B Ternary system at 873K and 1073 K, **Cheng Gang**

PB27 Next Generation CALPHAD Databases: Accurate approximation of the Debye model and its application for phase diagram calculations, **Roslyakova Irina**

PB28 The first principle calculation and experimental investigation of the $Ti_2(Al,Si)C$ solid solution, **Piven Kseniia**

PB29 Experimental and thermodynamic study of Li-O and Li_2O-P_2O_5 systems, **Jin Liling**

PB30 Thermodynamic description of spinodal decomposition in Ni-based superalloys, **Forghani Farsad**

PB31 Isothermal section of the Phase diagram of the Co-Pt-Ho ternary system at 773K, **Du Yusong**

PB32 Thermodynamic modelling of lead chalcogenide thermoelectrics for optimized ZT, **Peters Matthew**

PB33 Thermodynamic stability of substitutional- and interstitial-type of boron in fcc Fe, **Kouta Iyoda**

PB34 First-principles calculations and thermodynamic modeling of the Cu-Sn-S system relevant to CZTSSe photovoltaic materials, **Guan Pin-Wen**

PB35 Design of Ti-Alloy by Integrating High Throughput Experiments and Calculations, **Liu Libin**

PB36 ,

PB37 Phase relations of the Ce_2Co_{17}-Sm_2Co_{17} system, **Du Yusong**

PB38 Experimental reinvestigation and thermodynamic description of Bi-Te binary System, **Zhang Ligang**

PB39 Application of the CALPHAD approach and First-principles calculations to electrode materials in Li ion batteries, **Chang Keke**

PB40 Experimental investigation and thermodynamic modelling of LiF-NdF_3-DyF_3 system, **Abbasalizadeh Aida**

PB41 Thermodynamic properties of liquid In-Li solutions, **Gąsior Władysław**

PB42 Ab-initio study of finite pressure-temperature phase stability for magnetic materials, **Singh Harish Kumar**

PB43 Stability study of Ni_8V phase, **Noori Seyed-mohammad-mehdi**

PB44 Progress in the development of the OECD-NEA Thermodynamics Advanced Fuels - International Database (TAF-ID): Application calculations, **Guéneau Christine**

PB45 Assessment of NiO-SiO_2 System with Kapoor-Frohberg-Gaye Model, **Farina Alexandre**

PB46 Development of cemented carbides through thermodynamic calculations, **Peng Yingbiao**

PB47 Prediction of Free Energy at Finite Temperatures by First-Principles Calculations and Statistical Mechanics, **Liu Zi-Kui**

PB48 ,

PB49 Development of lightweight high entropy alloys using coupled CALPHAD-DFT modeling, **Huang Xuejun**

PB50 Thermodynamic modelling of FeO-Fe_2O_3-Ti_2O_3-TiO_2 system, **Panda Sourav Kumar**

PB51 Analysis at high lateral resolution of Mo-Ni-Re system with the CAMECA SXFIVE FE, **Robbes Anne-Sophie**

PB52 Thermodynamic properties of alloys of the binary Sb-Yb system, **Shevchenko Maksym**

PB53 Thermodynamic Assessment of Binary Subsystems of Al_2O_3-CaO-SiO_2-UO_2-ZrO_2 System Using Cell Model and Ionic Model, **Kurata Masaki**

PB54 Computational thermodynamics of solid-solid phase change materials development for thermal energy storage in ternary system: Pentaglycerine - Tris(hydroxymethyl)-aminomethane - 2-amino-2-methyl-1,3-propanediol (PG-TRIS-AMPL), **Chandra Dhanesh**

PB55 The 600°C isothermal section of the La-Zn-Si system, **Tu Hao**

PB56 Experimental investigation of the intermetallic dross phases formed in galvalume baths, **Peng Haoping**

PB57 Isothermal section of Zn-rich corner of the Zn-Al-Mg-Si system at 450° C, **Wang Jianhua**

PB58 High Temperature Experimental Contribution to the Thermodynamic Modeling of Corium Pools, **Gossé Stéphane**

PB59 Explicit calculations of vacancy profile during interdiffusion in quaternary Ni−Pt−Cr−Al system for optimization of new $\gamma - \gamma$ bond coating, **Desgranges Clara**

PB60 Mechanical Properties of Non-Centrosymmetric $CePt_3Si$ and $CePt_3B$, **Rogl Gerda**

PB61 Kinetic simulation of alloying element partitioning in Q&P steels, **Maheswari Nandakumar**