Views & Comments

View and Comments on the Data Ecosystem: "Ocean of Data"

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In a recent paper [1], I discussed the concept of the "ocean of data," in a response to ever-increasing computing power and large numbers of online data repositories. These settings call for a new paradigm of computational framework that connects various data repositories, incorporates machine learning, reuses existing data, and guides new computation and experimental efforts to create a "sustainable ecosystem" of data and tools. It is my hope that some recently available open-source codes can promote the development of pathways with lower barriers between individual data repositories and the ocean of data, and can add value to data processing in individual data repositories by communicating with the ocean of data, as schematically shown in Fig. 1 [1].

Thermodynamics is a science that concerns the state of a system—whether stable, metastable, or unstable—when interacting with the surroundings. The combination of the first and second laws of thermodynamics proposed by Gibbs [2,3] integrates the external and internal parts of a system. Even though Gibbs focused on the equilibrium of heterogeneous substances [2,4], the combined first and second laws of thermodynamics include both the equilibrium and non-equilibrium states of a system [5,6].

Thermodynamic modeling based on the calculation of phase diagram (CALPHAD) approach [6–9] establishes the Gibbs energy of individual phases across the complete space of the external and internal variables of the system, covering the stable, metastable, and unstable regions of each phase. In fact, the definition of the energy difference between the stable and non-stable structures of pure elements is the foundation of CALPHAD modeling, and was termed "lattice stability" by Kaufman, who pioneered the CALPHAD approach and coined the name [10,11]. The concept of lattice stability and the common acceptance of a set of lattice stability values have enabled the development of multicomponent databases with over 20 elements that have become the foundation of integrated computational materials engineering (ICME) [12] and the Materials Genome Initiative [13].

Before 2000, CALPHAD modeling relied almost exclusively on experimental information and some theoretical estimations, and its integration with the results from first-principles calculations based on density functional theory (DFT) [14] was rather limited [15]. The continued development of computation methods and software tools, particularly Vienna *ab-initio* simulation package (VASP) [16–18], has fueled the utilization of energetics from DFT-based first-principles calculations in CALPHAD modeling, and enabled the multidisciplinary information technology research

(ITR) project "Computational Tools for Multicomponent Materials Design" in 2002, which was supported by the US National Science Foundation (NSF). This ITR project integrated the DFT and CALPHAD approaches with phase-field simulations and finite-element methods [19]. The convergence of the DFT and CALPHAD methods along with the inspiration of the Human Genome Project [20] and the NSF-supported education program titled "An Integrated Education Program on Computational Thermodynamics, Kinetics, and Materials Design" [21] prompted me to coin the term "materials genome" in 2002 [22,23].

In 2009, I reviewed the first-principles calculations and CALPHAD modeling of thermodynamics [24]. My team established the extensible, self-optimizing phase equilibrium infrastructure (ESPEI) concept [25–27] that begins CALPHAD modeling using the thermochemical data of individual phases from first-principles calculations and refines model parameters using experimental phase equilibrium data. The significance of the ESPEI concept is threefold: ① First-principles calculations provide energetics as a function of internal degrees of freedom—that is, internally non-equilibrium configurations of each individual phase, which cannot be directly obtained from experiments because experimental data are usually for equilibrium states that are mixtures of many configurations [28–32]; ② ESPEI establishes a mechanism to efficiently evaluate model parameters, their statistic uncertainties, and uncertainty propagation in calculated properties [27,33]; and ③ the ESPEI data infrastructure integrates proto data and processed data from CALPHAD modeling and enables the efficient reuse of proto data and the effective updating and maintenance of processed data. With more and more publications on first-principles calculations, ubiquitous higher performance computing facilities, and large-scale online databases such as the Materials Project [34], open quantum materials database [35], and automatic flow for materials discovery [36] in the United States alone, I believe that the thermochemical data from DFT-based first-principles calculations will play an increasingly critical role in the CALPHAD modeling of a wide range of materials, particularly in the discovery and design of new materials.

Materials design based on CALPHAD databases, thermodynamic calculations, and kinetic simulations has been systemized by Olson for developing new materials and improving existing materials [37,38]. This materials design approach connects controllable parameters in processing with measurable quantities in properties using microstructure attributes. The key foundational variable
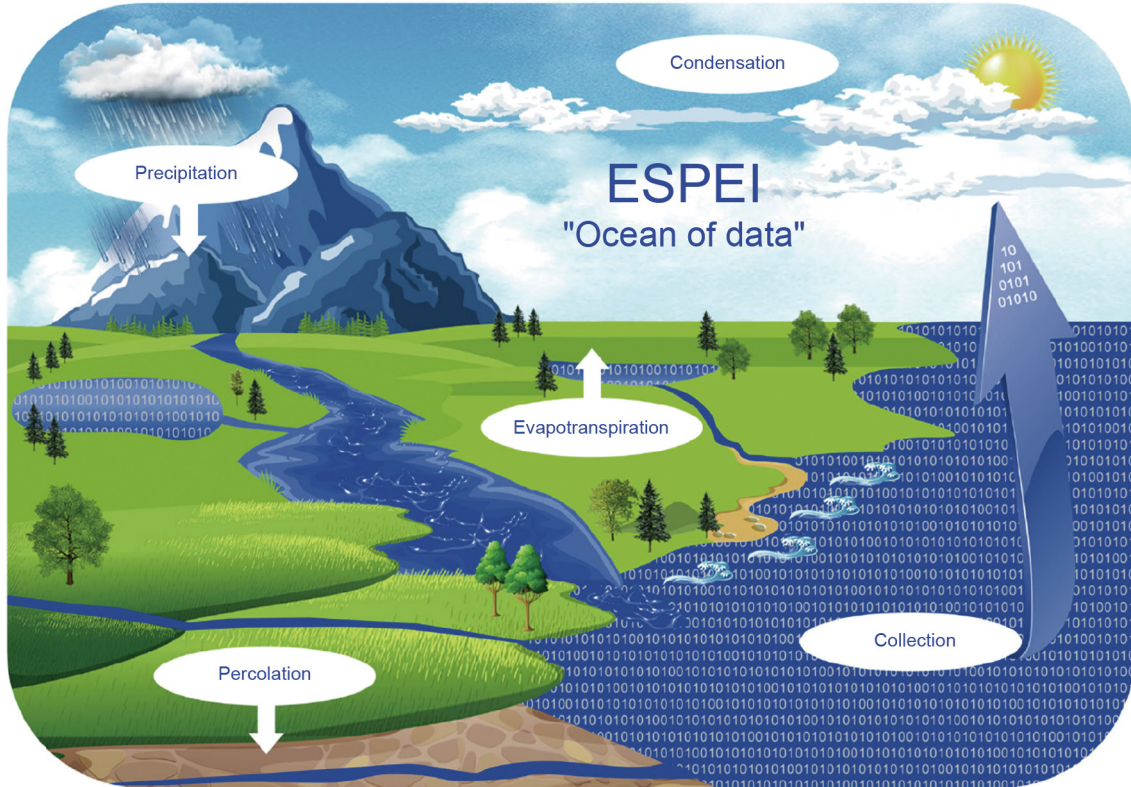
Fig. 1. Schematic diagram of a "sustainable ecosystem" of data showing various data repositories (lakes), interconnections (flows), private data (percolation), processing (evaporation), collection (ocean), and reuse (condensation and precipitation) [1]. ESPEI: extensible, self-optimizing phase equilibrium infrastructure.

among a plethora of microstructure attributes is the phases that are formed; this is in accordance with the modeling of individual phases in the CALPHAD approach, which has been extended to a range of other properties. Some examples by my research group are shown in Table 1 [28–32,39–69]. It may also be mentioned that the second derivatives of energy with respect to its natural variables represent many physical properties, as shown in Figs. 2 and 3 [6,13,70], in which some temporary terms are assigned to the derivatives last column and last row in Fig. 2 and last column plus the compress heat in Fig. 3.

Materials design is the first step of the life-cycle of materials. After design, materials are manufactured and put into service, both of which generate new proto data that enrich or contrast the existing proto and processed data. Furthermore, materials recycling is becoming critical for both environmental concerns and materials expenses. As recycling often involves several materials, the

Table 1
Examples of computed and modeled properties.

Properties	Examples
Thermal properties	Free energy [39,40], enthalpy, entropy, heat capacity, thermal expansion, and contraction [28–32]
Transport properties	Diffusion coefficient [41–43], Seebeck coefficient [44,45], and heat of transport [46,47]
Interfacial properties	Stacking fault energy [48–51], anti-phase boundary energy [52–54], grain boundary [48,55,56], and interfacial energy [57,58]
Elastic moduli	Refs. [59–61]
Dislocation properties	Refs. [62–64]
Magnetic properties	Refs. [28,29,65–67]
Relative creep rate	Ref. [43]
Other properties under development	Hardness, plasticity of single crystal [68,69]

chemistry of recycled materials can become more complex in comparison with the chemistry of the proto and processed data that were used to design each of the materials. These new proto data may thus necessitate additional first-principles calculations and the revision and expansion of processed data [71]. This is a critical connection for a sustainable data ecosystem, as shown in Fig. 4 [25–27,72–74], and it is a not trivial task, as current thermodynamic databases often contain more than 20 elements, albeit with limited proto data in the multidimensional space of external and internal variables [75–77]. It is my hope that our efforts in developing open-source software packages, DFTTK [78], pycalphad [72,73], and ESPEI [25–27,74] can inspire the community to develop new tools to further promote the materials research paradigm driven by science and computation [79].

Additional challenges are related to multiscale complexity in materials in terms of both length and time scales, and how information passes between scales to produce microscopic and macroscopic behaviors [19]. We have recently shown that the following entropy equations hold promise for multiscale integrations of materials' properties and information through entropy [80]:

$$S = \sum_{k=1}^{m} p^k \left(S^k - k_B \ln p^k \right) \tag{1}$$

$$dS = \frac{dQ}{T} + \sum S_j dN_j + d_{IP}S \tag{2}$$

$$d_{IP}S = \frac{d_{IP}Q}{T} - \sum S_j^n dN_j^n + \sum S_l^w dN_l^w - d_{IP}I \tag{3}$$

Eq. (1) represents the total entropy of a system, S, calculated from the configurations at the scale k, with p^k being the probability of configuration $k \in \{1, ..., m\}$ of the system and $\sum_{k=1}^{m} p^k = 1$, S^k being the entropy of each configuration in the scale k, and k_B

	Temperature (T)	Stress (σ_{kl})	Electric field (E_k)	Magnetic field (H_k)	Chemical potential (μ_k)
Entropy (S)	Heat capacity (C_V/T)	Piezocaloric effect (α_{kl})	Electrocaloric effect (p_x)	Magnetocaloric effect (m_k)	Entropic diffusion ($\frac{\partial \mu_k}{\partial S}$)
Strain (ε_{ij})	Thermal expansion (α_{ij})	Elastic compliance (s_{ijkl})	Converse piezoelectricity (d_{ijk})	Piezomagnetic moduli (q_{ijk})	Strain diffusion ($\frac{\partial \mu_k}{\partial \varepsilon_{ij}}$)
Electric displacement (D_i)	Pyroelectric coefficients (p_i)	Piezoelectric moduli (d_{ikl})	Permittivity (k_{ik})	Magnetoelectric coefficient (a_{ik})	Electric diffusion ($\frac{\partial \mu_k}{\partial D_i}$)
Magnetic induction (B_i)	Pyromagnetic coefficient (m_i)	Piezomagnetic moduli (q_{ikl})	Magnetoelectric coefficient (a_{ik})	Permeability (μ_{ik})	Magnetic diffusion ($\frac{\partial \mu_k}{\partial B_i}$)
Moles (N_i)	Thermal mass ($\frac{\partial N_i}{\partial T}$)	Stress mass ($\frac{\partial N_i}{\partial \sigma_{kl}}$)	Electric mass ($\frac{\partial N_i}{\partial E_k}$)	Magnetic mass ($\frac{\partial N_i}{\partial H_k}$)	Thermodynamic factor ($\frac{\partial \mu_k}{\partial N_i}$)

Fig. 2. Physical quantities related to the second directives of internal energy with respect to its natural variables [6,13].

	Entropy (S)	Volume (V)	Chemical potential (μ_k)
Temperature (T)	Heat capacity ($-\frac{\partial S}{\partial T} = -C_p T$)	Thermal expansion ($\frac{\partial V}{\partial T}$)	Thermal transport ($\frac{\partial \mu_k}{\partial T}$)
Pressure (P)	Compress heat ($-\frac{\partial S}{\partial P}$)	Compressibility ($\frac{\partial V}{\partial P}$)	Compress diffusion ($\frac{\partial \mu_k}{\partial P}$)
Moles (N_i)	Partial molar entropy ($-S_i = -\frac{\partial S}{\partial N_i}$)	Partial molar volume ($V_i = \frac{\partial V}{\partial N_i}$)	Thermodynamic factor ($\frac{\partial \mu_k}{\partial N_i}$)

Fig. 3. Physical quantities related to the second directives of Gibbs energy with respect to its natural variables [70].
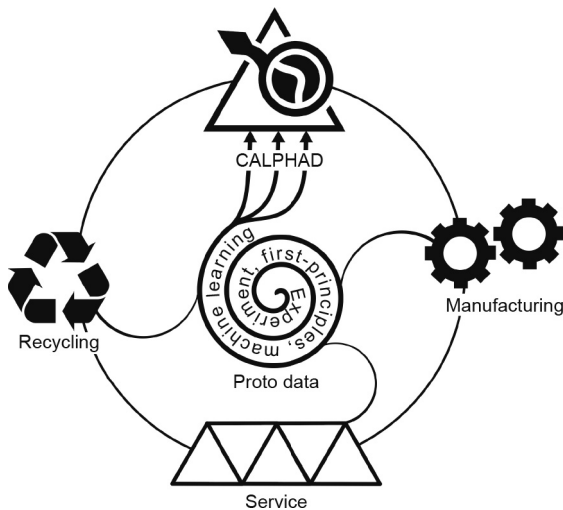

Fig. 4. Schematic chart of the data ecosystem including proto data (experiment, first-principles calculations, and machine learning), processed data (modeling: CALPHAD with pycalphad [72,73] and ESPEI [25–27,74]), materials manufacturing, materials service, and materials recycling.

representing the Boltzmann constant. It is important to note that the entropy of the system consists of the configurational entropy at the scale of consideration plus the entropy of each individual configuration, and the probability of each configuration is related to the free energies of all configurations. Each individual configuration itself consists of another set of configurations, and S^k can thus be expressed in the same form as Eq. (1) with its own configurations. This division can continue until all important scales are considered. In the domain of materials science and engineering, where the focus is on the formation of phases, the atomic configurations represent the dominant scale with subscales of electronic and phonon density of states [39].

In Eq. (2), dS is the entropy change of the system, dQ is the amount of heat that the system receives from the surroundings,

S_j is the partial molar entropy of component j in the surroundings or the system, dN_j is the amount of component j that the system receives from (d$N_j > 0$) or releases to the surroundings (d$N_j < 0$), T is the temperature, and d$_{IP}S$ is the entropy production due to independent internal processes (IP). The first term on the right-hand side of the equation is often how the concept of entropy is introduced in the thermodynamics of materials, while the second term is not discussed very much and is often buried in the direct introduction of chemical potential into the combined first and second laws of thermodynamics. The details of the third term, entropy production, are typically considered as part of kinetics and are not addressed in thermodynamics due to the usual consideration of equilibrium states only. It is worth noting that the entropy in the combined first and second laws of thermodynamics contains all three terms in Eq. (2) though often not explicitly stated [80].

Eq. (3) shows that the entropy production due to an internal process can be written in a similar form as Eq. (2) by defining the internal process as an IP-system [80]. This IP-system may consume some nutrients $\left(dN_j^n\right)$ with partial entropy of S_j^n, generate some waste $\left(dN_l^w\right)$ with partial entropy of S_l^w, produce heat (d$_{IP}Q$), and reorganize its configurations to produce a certain amount of information (d$_{IP}I$), which can be written as follows using Eq. (1):

$$d_{IP}I = -(S_f - S_i) = \sum_{k_i=1}^{m_i} p^{k_i}\left(S^{k_i} - k_B \ln p^{k_i}\right)$$
$$- \sum_{k_f=1}^{m_f} p^{k_f}\left(S^{k_f} - k_B \ln p^{k_f}\right) \qquad (4)$$

where the subscripts f and i represent the final and initial configurations of the IP-system. For a spontaneous/irreversible internal process, the entropy production represented by Eq. (3) must be positive, based on the second law of thermodynamics; however, the sign of d$_{IP}I$ can be either positive (generate information) or negative (erase information). Various thought experiments are discussed in Ref. [80]. It should be noted that the sign conventions in Eqs. (2) and (3) are opposite, with a positive sign indicating

that a system receives heat and mass from the surroundings in Eq. (2), but indicating that an IP-system gives out heat and mass in Eq. (3) as they increase the entropy.

CALPHAD modeling based on the properties of individual phases has proven to be foundational for computational materials science and engineering. To further enhance the predictive power of the CALPHAD method, I suggest including configurations at relevant scales as shown by Eq. (1), so properties at various scales can be predicted, including the emergent behaviors that individual configurations do not possess. Extreme emergent behavior is observed in relation to the limit of the stability of a system when the derivative of temperature to entropy approaches zero from a positive value in its stable region [6]. Consequently, the derivative of entropy to temperature becomes positive infinite because temperature and entropy are conjugate variables in the combined law of thermodynamics—that is, the entropy change diverges, resulting from competition among the stable and metastable configurations shown by Eq. (1). It should be noted that not only is this divergence of the entropy of the system not a behavior that each individual configuration possesses, but also all molar, extensive quantities of the system diverge at the limit of stability. Furthermore, they may diverge negatively, such as thermal expansion represented by the derivative of volume to temperature, because volume and temperature are not conjugate variables in the combined law of thermodynamics [6]. This has been demonstrated by us for cerium, with a positive divergence, and for Fe_3Pt, with a negative divergence, in terms of thermal expansion [28–30]. It should also be noted that the derivative of volume to temperature is equal to the negative derivative of entropy to pressure which is named as "compress heat," due to the Maxwell relations [6] so the quantities in Figs 2 and 3 in the present article are symmetrical.

References

[1] Liu ZK. Ocean of data: integrating first-principles calculations and CALPHAD modeling with machine learning. J Phase Equilibria Diffus 2018;39(5):635–49.

[2] Gibbs JW. The collected works of J. Willard Gibbs: vol. I. thermodynamics. New Haven: Yale University Press; 1948.

[3] Gibbs JW. The collected works of J. Willard Gibbs: vol. II. statistical mechanics. New Heaven: Yale University Press; 1948.

[4] Gibbs JW. On the equilibrium of heterogeneous substances. Am J Sci 1878;16(3):441–58.

[5] Hillert M. Phase equilibria, phase diagrams and phase transformations: their thermodynamic basis. 2nd ed. Cambridge: Cambridge University Press; 2008.

[6] Liu ZK, Wang Y. Computational thermodynamics of materials. Cambridge: Cambridge University Press; 2016.

[7] Kaufman L, Bernstein H. Computer calculation of phase diagrams with special reference to refractory metals. New York: Academic Press Inc; 1970.

[8] Saunders N, Miodownik AP. CALPHAD (calculation of phase diagrams): a comprehensive guide. Oxford: Pergamon; 1998.

[9] Lukas HL, Fries SG, Sundman B. Computational thermodynamics: the CALPHAD method. Cambridge: Cambridge University Press; 2007.

[10] Kaufman L. The lattice stability of metals—I. titanium and zirconium. Acta Metall 1959;7(8):575–87.

[11] Kaufman L. The lattice stability of the transition metal. In: Rudman PS, Stringer JS, Jaffee RI, editors. Phase stability in metals and alloys. New York: McGraw-Hill; 1967. p. 125–50.

[12] National Research Council. Integrated computational materials engineering: a transformational discipline for improved competitiveness and national security. Washington, DC: The National Academies Press; 2008.

[13] National Science and Technology Council. Materials Genome Initiative for global competitiveness [Internet]. Washington, DC: National Science and Technology Council; 2011 Jun 24 [cited 2017 Mar 22]. Available from: https://www.mgi.gov/sites/default/files/documents/materials_genome_initiative-final.pdf.

[14] Kohn W, Sham LJ. Self-consistent equations including exchange and correlation effects. Phys Rev 1965;140(4A):1133–8.

[15] Spencer PJ. A brief history of CALPHAD. Calphad 2008;32(1):1–8.

[16] Hafner J, Sommer F. *Ab-initio* pseudopotential calculations of the structure and stability of binary alloys and intermetallic compounds. Calphad 1977;1(4):325–40.

[17] Kresse G, Hafner J. *Ab initio* molecular dynamics for open-shell transition metals. Phys Rev B Condens Matter 1993;48(17):13115–8.

[18] Hafner J. *Ab-initio* simulations of materials using VASP: density-functional theory and beyond. J Comput Chem 2008;29(13):2044–78.

[19] Liu ZK, Chen LQ, Raghavan P, Du Q, Sofo J, Langer SA, et al. An integrated framework for multi-scale materials simulation and design. J Comput Mater Des 2004;11(2–3):183–99.

[20] National Human Genome Research Institute. The Human Genome Project [Internet]. Bethesda: National Institutes of Health; [cited 2018 Jun 26]. Available from: https://www.genome.gov/10001772/all-about-the–human-genome-project-hgp/.

[21] Liu ZK, Chen LQ, Spear KE, Pollard C. An integrated education program on computational thermodynamics, kinetics, and materials design [Internet]. Warrendale: The Minerals, Metals & Materials Society; c2003 [cited 2019 Jan 13]. Available from: https://www.tms.org/pubs/journals/JOM/0312/LiuII/LiuII-0312.html.

[22] Liu ZK. Perspective on materials genome. Chin Sci Bull 2013;58(35):3618–22. Chinese.

[23] Liu ZK. Perspective on materials genome®. Chin Sci Bull 2014;59(15):1619–23.

[24] Liu ZK. First-principles calculations and CALPHAD modeling of thermodynamics. J Phase Equilibria Diffus 2009;30(5):517–34.

[25] Shang SL, Wang Y, Liu ZK. ESPEI: extensible, self-optimizing phase equilibrium infrastructure for magnesium alloys. In: Proceedings of the Magnesium Technology 2010—TMS 2010 Annual Meeting and Exhibition; 2010 Feb 14–18; Seattle, WA, USA; 2010. p. 617–22.

[26] Otis RA, Liu ZK. High-throughput thermodynamic modeling and uncertainty quantification for ICME. JOM 2017;69(5):886–92.

[27] Bocklund BJ, Otis R, Egorov A, Obaied A, Roslyakova I, Liu ZK. ESPEI for efficient thermodynamic database development, modification, and uncertainty quantification: application to Cu–Mg. MRS Commun 2019;9(2):618–27.

[28] Wang Y, Hector Jr LG, Zhang H, Shang SL, Chen LQ, Liu ZK. Thermodynamics of the Ce γ–α transition: density-functional study. Phys Rev B 2008;78 104113.

[29] Wang Y, Shang SL, Zhang H, Chen LQ, Liu ZK. Thermodynamic fluctuations in magnetic states: Fe_3Pt as a prototype. Philos Mag Lett 2010;90(12):851–9.

[30] Liu ZK, Wang Y, Shang S. Thermal expansion anomaly regulated by entropy. Sci Rep 2014;4(1):7043.

[31] Liu ZK, Wang Y, Shang SL. Origin of negative thermal expansion phenomenon in solids. Scr Mater 2011;65(2):664–7.

[32] Liu ZK, Shang SL, Wang Y. Fundamentals of thermal expansion and thermal contraction. Materials 2017;10(4):410.

[33] Paulson NH, Bocklund BJ, Otis RA, Liu ZK, Stan M. Quantified uncertainty in thermodynamic modeling for materials design. Acta Mater 2019;174:9–15.

[34] The materials project [Internet]. [cited 2019 Jan 13]. Available from: http://materialsproject.org/.

[35] OQMD. The open quantum materials database [Internet]. [cited 2019 Jan 13]. Available from: http://oqmd.org.

[36] AFLOW. Automatic flow for materials discovery [Internet]. [cited 2019 Jan 13]. Available from: http://www.aflowlib.org.

[37] Olson GB. Computational design of hierarchically structured materials. Science 1997;277(5330):1237–42.

[38] Olson GB, Kuehmann CJ. Materials genomics: from CALPHAD to flight. Scr Mater 2014;70:25–30.

[39] Wang Y, Liu ZK, Chen LQ. Thermodynamic properties of Al, Ni, NiAl, and Ni_3Al from first-principles calculations. Acta Mater 2004;52(9):2665–71.

[40] Shang SL, Wang Y, Kim D, Liu ZK. First-principles thermodynamics from phonon and Debye model: application to Ni and Ni_3Al. Comput Mater Sci 2010;47(4):1040–8.

[41] Mantina M, Wang Y, Arróyave R, Chen LQ, Liu ZK, Wolverton C. First-principles calculation of self-diffusion coefficients. Phys Rev Lett 2008;100(21):215901.

[42] Zhou BC, Shang SL, Wang Y, Liu ZK. Diffusion coefficients of alloying elements in dilute Mg alloys: a comprehensive first-principles study. Acta Mater 2016;103:573–86.

[43] Hargather CZ, Shang SL, Liu ZK. Electronic structures and materials properties calculations of Ni and Ni-based superalloys. In: Horstemeyer MF, editor. Integrated computational materials engineering (ICME) for metals: concepts and case studies. Hoboken: John Wiley & Sons; 2018. p. 413–46.

[44] Wang Y, Hu YJ, Bocklund B, Shang SL, Zhou BC, Liu ZK, et al. First-principles thermodynamic theory of Seebeck coefficients. Phys Rev B 2018;98(22):224101.

[45] Wang Y, Chong X, Hu YJ, Shang SL, Drymiotis FR, Firdosy SA, et al. An alternative approach to predict Seebeck coefficients: application to $La_{3-x}Te_4$. Scr Mater 2019;169:87–91.

[46] Evteev AV, Levchenko EV, Belova IV, Kozubski R, Liu ZK, Murch GE. Thermotransport in binary system: case study on $Ni_{50}Al_{50}$ melt. Philos Mag 2014;94(31):3574–602.

[47] Sarder U, Ahmed T, Wang WY, Kozubski R, Liu ZK, Belova IV, et al. Mass and thermal transport in liquid Cu–Ag alloys. Philos Mag 2019;99(4):468–91.

[48] Wang Y, Chen LQ, Liu ZK, Mathaudhu SN. First-principles calculations of twin-boundary and stacking-fault energies in magnesium. Scr Mater 2010;62(9):646–9.

[49] Shang SL, Wang WY, Wang Y, Du Y, Zhang JX, Patel AD, et al. Temperature-dependent ideal strength and stacking fault energy of fcc Ni: a first-principles study of shear deformation. J Phys Condens Matter 2012;24(15):155402.

[50] Wang WY, Shang SL, Wang Y, Mei ZG, Darling KA, Kecskes LJ, et al. Effects of alloying elements on stacking fault energies and electronic structures of binary Mg alloys: a first-principles study. Mater Res Lett 2014;2(1):29–36.

[51] Hargather CZ, Shang SL, Liu ZK. A comprehensive first-principles study of solute elements in dilute Ni alloys: diffusion coefficients and their implications to tailor creep rate. Acta Mater 2018;157:126–41.

[52] Manga VR, Saal JE, Wang Y, Crespi VH, Liu ZK. Magnetic perturbation and associated energies of the antiphase boundaries in ordered Ni$_3$Al. J Appl Phys 2010;108(10):103509.

[53] Manga VR, Shang SL, Wang WY, Wang Y, Liang J, Crespi VH, et al. Anomalous phonon stiffening associated with the (111) antiphase boundary in L1$_2$Ni$_3$Al. Acta Mater 2015;82:287–94.

[54] Wang WY, Xue F, Zhang Y, Shang SL, Wang Y, Darling KA, et al. Atomic and electronic basis for solutes strengthened (010) anti-phase boundary of L1$_2$Co$_3$(Al,TM): a comprehensive first-principles study. Acta Mater 2018;145:30–40.

[55] Fang HZ, Wang Y, Shang SL, Jablonski PD, Liu ZK. First-principles calculations of interfacial and segregation energies in α-Cr$_2$O$_3$. J Phys Condens Matter 2012;24(22):225001.

[56] Wang WY, Shang SL, Wang Y, Hu YJ, Darling KA, Kecskes LJ, et al. Lattice distortion induced anomalous ferromagnetism and electronic structure in fcc Fe and Fe–TM (TM = Cr, Ni, Ta and Zr) alloys. Mater Chem Phys 2015;162:748–56.

[57] Wang Y, Liu ZK, Chen LQ, Wolverton C. First-principles calculations of β''-Mg$_5$Si$_6$/α-Al interfaces. Acta Mater 2007;55(17):5934–47.

[58] Liu XL, Shang SL, Hu YJ, Wang Y, Du Y, Liu ZK. Insight into γ-Ni/γ'-Ni$_3$Al interfacial energy affected by alloying elements. Mater Des 2017;133: 39–46.

[59] Shang SL, Wang Y, Liu ZK. First-principles elastic constants of α- and θ-Al$_2$O$_3$. Appl Phys Lett 2007;90(10):101909.

[60] Shang SL, Zhang H, Wang Y, Liu ZK. Temperature-dependent elastic stiffness constants of α- and θ-Al$_2$O$_3$ from first-principles calculations. J Phys Condens Matter 2010;22(37):375403.

[61] Liu ZK, Zhang H, Ganeshan S, Wang Y, Mathaudhu SN. Computational modeling of effects of alloying elements on elastic coefficients. Scr Mater 2010;63(7):686–91.

[62] Hu YJ, Fellinger MR, Butler BG, Wang Y, Darling KA, Kecskes LJ, et al. Solute-induced solid-solution softening and hardening in bcc tungsten. Acta Mater 2017;141:304–16.

[63] Zhang SH, Beyerlein IJ, Legut D, Fu ZH, Zhang Z, Shang SL, et al. Effect of strain on the stacking fault energies, dislocation core structure and Peierls stress of magnesium and its alloys. Phys Rev B 2017;95:224106.

[64] Shang SL, Shimanek J, Qin SP, Wang Y, Beese AM, Liu ZK. Unveiling dislocation characteristics in Ni$_3$Al from stacking fault energy and ideal strength: a first-principles study via pure alias shear deformation. Phys Rev B 2020;101:024102.

[65] Wang Y, Hector Jr LG, Zhang H, Shang S, Chen LQ, Liu ZK. A thermodynamic framework for a system with itinerant-electron magnetism. J Phys Condens Matter 2009;21(32):326003.

[66] Shang SL, Wang Y, Liu ZK. Thermodynamic fluctuations between magnetic states from first-principles phonon calculations: the case of bcc Fe. Phys Rev B 2010;82(1):014425.

[67] Shang SL, Saal JE, Mei ZG, Wang Y, Liu ZK. Magnetic thermodynamics of fcc Ni from first-principles partition function approach. J Appl Phys 2010;108 (12):123514.

[68] Kim H. Thermodynamic modeling and mechanical properties modeling of Long Periodic Stacking Ordered (LPSO) phases [dissertation]. University Park: Pennsylvania State University; 2019.

[69] Qin S, Shang SL, Shimanek J, Liu ZK, Beese AM. Macroscopic plastic deformation through an integrated first-principles calculations and finite element simulations: application to nickel single crystal. 2020. arXiv:2002.08552.

[70] Liu ZK. Computational thermodynamics and its applications. Acta Mater 2020. In press.

[71] Campbell CE, Kattner UR, Liu ZK. File and data repositories for next generation CALPHAD. Scr Mater 2014;70:7–11.

[72] Otis RA, Liu ZK. Pycalphad: CALPHAD-based computational thermodynamics in Python. J Open Res Softw 2017;5(1):1.

[73] Pycalphad: computational thermodynamics [Internet]. c2015 [cited 2017 Jul 20]. Available from: http://pycalphad.org.

[74] ESPEI: extensible self-optimizing phase equilibria infrastructure [Internet]. c2018–2019 [cited 2018 Apr 11]. Available from: http://espei.org.

[75] Databases [Internet]. Solna: Thermo-Calc Software; [cited 2019 Jan 13]. Available from: https://www.thermocalc.com/products-services/databases/.

[76] FactSage 7.3—summary of databases [Internet]. [cited 2019 Jan 13]. Available from: http://www.crct.polymtl.ca/fact/documentation/FSData.htm.

[77] CompuTherm databases [Internet]. Middleton: CompuTherm LLC; [cited 2019 Jan 13]. Available from: http://www.computherm.com/index.php?route= product/category&path=59.

[78] DFTTK: density functional theory tool kits [Internet]. San Francisco: The GitHub; c2020 [cited 2019 Jan 13]. Available from: https://github.com/ PhasesResearchLab/dfttk.

[79] Liu ZK. A materials research paradigm driven by computation. JOM 2009;61 (10):18–20.

[80] Liu ZK, Li B, Lin H. Multiscale entropy and its implications to critical phenomena, emergent behaviors, and information. J Phase Equilibria Diffus 2019;40(4):508–21.