

## SCIENCE POLICY

Special Topic: Computational Materials and Multiscale Systems

**Mesoscience: exploring the common principle at mesoscales**Wenlai Huang<sup>1</sup>, Jinghai Li<sup>1,\*</sup> and Peter P. Edwards<sup>2</sup>**BACKGROUND OF THE EMERGING MESOSCIENCE**

In studying a complex system in science, engineering or society, we usually observe its macroscale (system-scale) behavior first, then go deep into mechanisms at the microscale (unit-scale) and finally try to correlate these two scales to reach a complete understanding. However, it is increasingly recognized that correlating these two scales is quite difficult, and some common principles are inevitably missing in between these two extrema [1,2].

For instance, in life science, genomics has been established through resolving the gene-scale while many radical issues of life are still challenging. Similarly, in the study of turbulence, with increasing understanding and emphasis towards smaller scales, much finer eddy structures are successively involved in various turbulence models, in which more parameters are incorporated, but how to unify such models is still pending. Another example is the design of materials. Although the atomic structures of all the chemical elements are understood, it is still highly challenging to design a material of specific interest, since there is, as yet, no definite and accepted route to follow. In chemical engineering, descriptions of a single particle, including its motion, transport and reaction processes, have long been available, even in textbooks, but quantitatively designing, scaling up and optimizing a complete working reactor is still a dream. In cognitive science, neurons and sensors over the whole body are explored in detail, and it is known that the brain makes decisions based on all signals received from them. However, due to limited understanding on the multi-level, multiscale nature and especially the

mesoscale complexity at each level in the neural system, cognitive science is still immature. Similar examples exist across almost all fields.

On the other hand, it is unrealistic, at least currently, to understand the behavior of a system through capturing all the microscale details in the whole system. Therefore, effectively correlating microscales with macroscales in studying complex systems by understanding the governing principles at the mesoscales is a common challenge, seriously restricting our capability of handling genuinely global challenges, most notably to realize sustainable development.

Our study in the past three decades has progressively revealed that the difficulty in correlating microscales with macroscales lies in the fact that a governing principle at mesoscales in between has so far been neglected. This principle is probably governed by ‘Compromise-in-competition between different dominant mechanisms’, called the EMMS (Energy Minimization Multi-Scale) principle [3,4]. It is gradually being recognized that this is the missing principle that makes the understanding of the spatiotemporally dynamic mesoscale structures such a challenge. Therefore, the transdisciplinary concept of mesoscience has been proposed [1,2,5,6].

Mesoscale herewith refers to a range of scale in between the micro- (element) scale and the macro- (system) scale and, within this range of scale, a characteristic structure exists, namely meso-structure, featuring dynamic heterogeneity in space and time, which is critical to the performance of the system. Parameters at the mesoscale are needed to bridge the mechanism at the element scale to the behavior of the system. The objective of

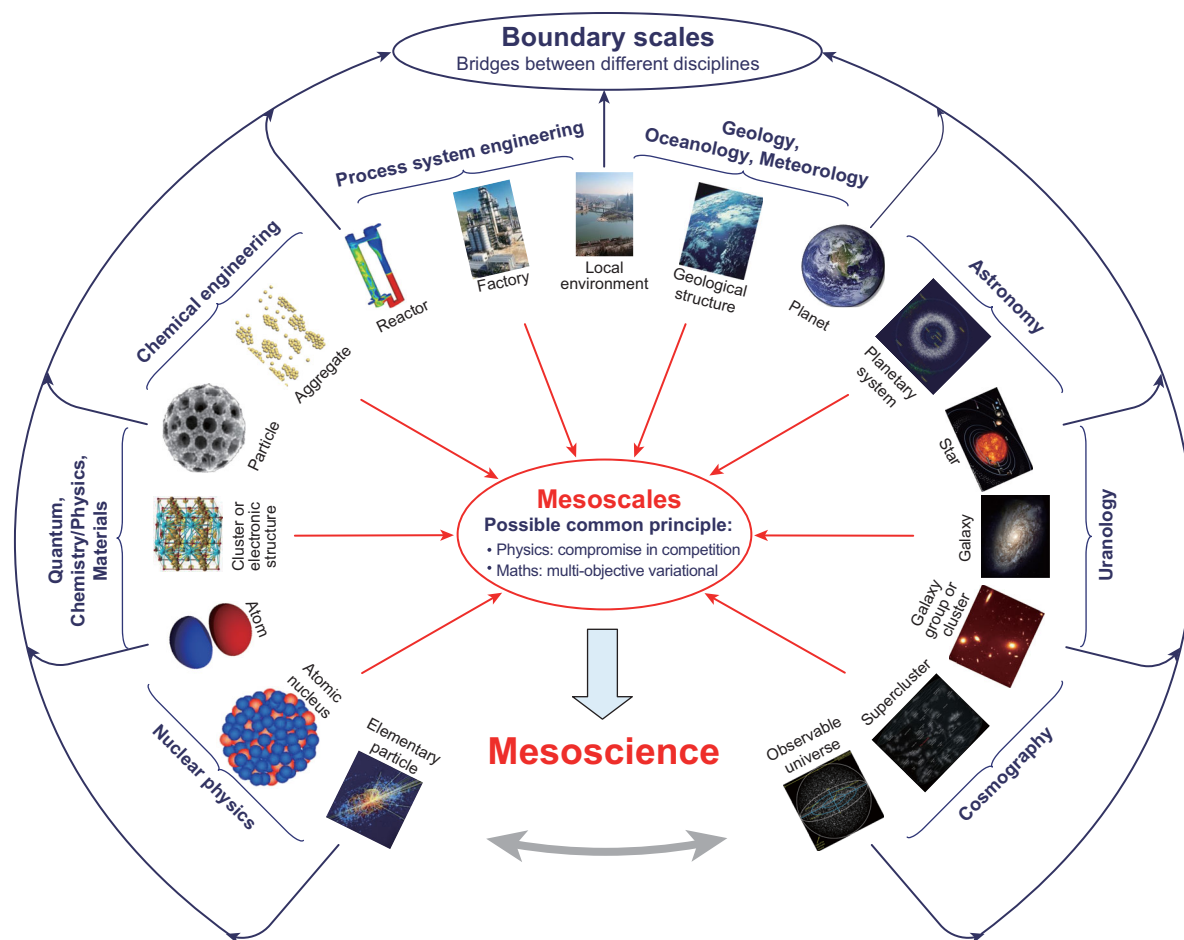
mesoscience is to develop a principle as general as possible to make such a bridge for different levels of disciplines, as shown in Fig. 1 [6].

The Natural Science Foundation of China (NSFC) initiated a mesoscience program entitled ‘Mechanism and manipulation at mesoscales in multiphase reaction processes’ in 2012 [7]. The program aims to understand various mesoscale issues at the two different levels (materials and reactors) in chemical engineering in order to look for common rules related to mesoscience.

Considering the ubiquity of mesoscale issues, however, the importance of mesoscience extends far beyond chemical engineering. In fact, our real world exhibits a multi-level nature, the structures at each level are all multiscale and the complexity appears likely at its mesoscale [8,9]. The development of mesoscience will enable each discipline to tackle complex issues, and therefore deserves great attention from the whole spectrum of science and engineering.

**POSSIBLE UNIVERSALITY OF MESOSCIENCE**

The concept of mesoscience arose from our exploration of complex systems in chemical engineering [4,10,11]. Typically, in gas-solid fluidized systems, at the mesoscale between the particle scale and the whole reactor scale, particle clusters or gas bubbles exist inherently. Investigations on these mesoscale phenomena revealed that they originate from the fact that the particles tend to minimize their potential energy, i.e. the average voidage  $\varepsilon \rightarrow \min$ , and, meanwhile, the gas tends to pass the



**Figure 1.** A unified theory of mesoscience will encompass all mesoscale phenomena: this represents a common challenge for the whole spectrum of science and technology. Modified from [6].

particles layer with minimum resistance, i.e. the rate of energy consumption with respect to unit volume for transporting suspending particles  $W_{st} \rightarrow \min$  [4]. Eventually, these two dominant mechanisms compromise in competition and realize their tendencies alternately with respect to space and time, leading to complex spatiotemporal structures at the mesoscale. With the change in specified conditions, the relative dominance of the two mechanisms varies, and three regimes with completely different features may appear successively, i.e. A-dominated, A-B compromising and B-dominated, as illustrated in Fig. 2 [8]. This regime-specific nature gives the rationale to use the term mesoscience, instead of mesoscale science, since complexity occurs

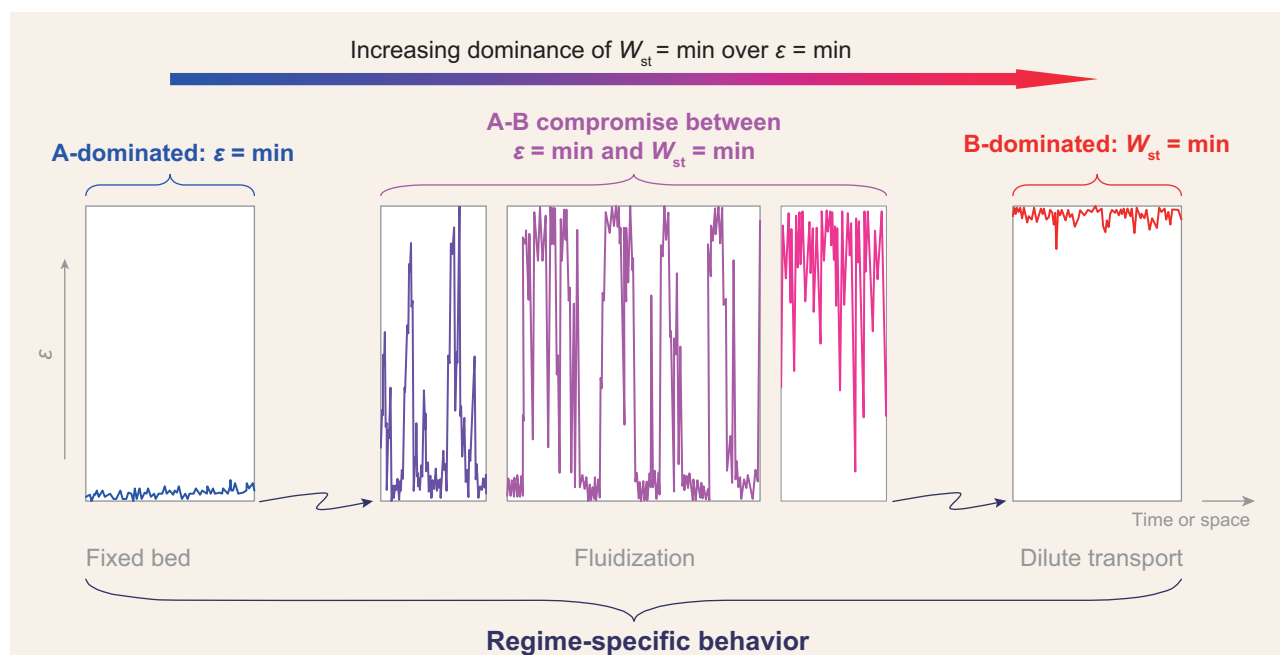
at mesoscales in mesoregimes with respect to different levels. Both mesoscales and mesoregimes are substantial to mesoscience.

A follow-up study on turbulent pipe flow unraveled that turbulence also results from the compromise in competition between the minimization of viscous dissipation and the maximization of inertial dissipation [12,13]. These two extreme cases alternately dominate with respect to both time and space, and in the middle regime between them, resulting in turbulence.

These two case studies led to the proposition of the EMMS principle of compromise in competition, formulated as a multi-objective variational problem, as given in Equation (1) [4], which has been verified in more systems [10].

$$\min \begin{pmatrix} E_1(\mathbf{X}) \\ \vdots \\ E_k(\mathbf{X}) \end{pmatrix}, \text{ s.t. } F_j(\mathbf{X}) = 0 \quad (1)$$

In Equation (1),  $\mathbf{X}$  is the structural vector (a set of structural variables) including parameters at three scales,  $E_i(\mathbf{X})$  ( $i = 1, \dots, k$ , and  $k = 2$  in the above two cases) is the  $i$ th variational function (corresponding to the  $i$ th dominant mechanism) and  $F_j(\mathbf{X}) = 0$  ( $j = 1, \dots, m$ ) is the  $j$ th conservation equation. When the parameters at the system scale are heterogeneously distributed, such as radial distribution usually encountered in chemical reactors, the treatment could be even more complicated [1].



**Figure 2.** Three regimes that occur successively as the relative dominance of mechanism B over mechanism A changes and the evolution of structures in the A-B compromising regime. Modified from [8].

In recent years, this principle was verified further in heterogeneous catalysis [14], protein folding [15], etc., providing additional evidence for the possible generality of the principle and enabling the proposition of mesoscience [1,2,5,6,8,9,16–20].

### MORE EVIDENCE NEEDED TO VERIFY THE UNIVERSALITY OF MESOSCIENCE

Owing to the diversity and complexity, especially the level-specific and regime-specific features [8,9] of mesoscale phenomena, directly formulating a general theory for mesoscience through theoretical approaches will be formidable, though not inconceivable. This possibly is the reason why complexity science and non-equilibrium thermodynamics have not made breakthroughs over several decades.

Encouraged by our three-decade exploration on various complex multiphase systems, we believe that an effective approach to developing mesoscience might be through investigating a range of different mesoscale issues, identifying common rules from diversity, and thus

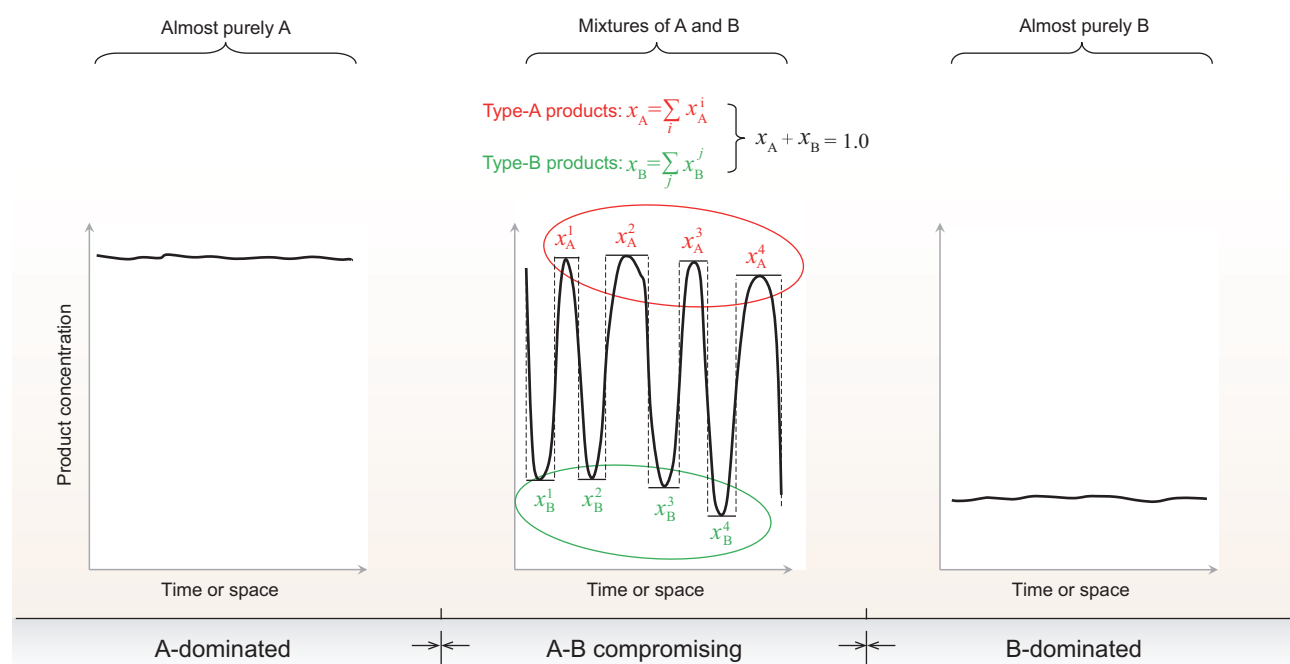
modifying and confirming the principle of compromise in competition. According to some clues collected previously, the following problems, as case studies, deserve close efforts in the near future:

- (i) **Selectivity in complex reactive systems.** Under specified conditions (temperature, pressure/concentrations, catalysts, etc.), reactants undertake various kinetic processes (diffusion, adsorption, desorption, reactions, etc.) and generate different products through different pathways in complex reactive systems. From our perspective, different pathways might correspond to different dominant mechanisms, and one dominant mechanism leads to one type of product. Therefore, changing the relative dominance of different mechanisms will lead to the change in product constituents, i.e. the conversion, yield and selectivity, as illustrated in Fig. 3. Assuming there are two kinds of products, A and B, corresponding to two mechanisms (denoted as A and B, respectively, as well), tailoring the relative dominance

of these two mechanisms will lead to three regimes (Fig. 3).

In Fig. 3,  $x_A$  and  $x_B$  are the conversions of products A and B, respectively. The present analysis is certainly oversimplified, but it might be a preliminary guideline. This idea has been preliminarily confirmed in a reactive system of toluene to benzonitrile and benzamide [21], and further study will benefit both mesoscience and the understanding of complex reactive systems.

- (ii) **Metal-nonmetal transition.** Such an electronic phase transition of nonmetal-to-metal can occur in countless systems, including doped semiconductors, metal-ammonia solutions, metal clusters or wires, etc., with the changes in the dopant concentration, the metal concentration, the relevant size, etc., respectively [22]. Roughly speaking, under a fixed current (or voltage), the metallic state will correspond to the minimum (or maximum) dissipation while the nonmetallic state exhibits the maximum (or minimum) dissipation. Importantly, the intermediate regime might



**Figure 3.** Three-regime prediction of the mechanisms in reactive systems.

show a combination of these two canonical end states [23], featuring the alternate occurrence of minimization and maximization of dissipation locally in space or time, e.g. the conductivity fluctuations, reflecting the inevitable compromise between these two regimes at the mesoscale. Such a compromise between minimization and maximization of dissipation has been confirmed in other fields such as gas-solid fluidization [9], turbulence [13] and catalysis [16]. The width of such an intermediate, compromising regime may be critically dependent on other conditions, e.g. the temperature.

- (iii) **Crystallization.** Depending on the specified conditions during crystallization, three regimes might also appear: the A-dominated regime where the crystallinity reaches 100% at the idealized condition, the B-dominated regime where the product is completely amorphous, and the middle regime in between where crystals and ‘non-crystals’ coexist, reflecting the compromise between mechanism A and mechanism B. Such non-crystals might be characterized as various complex

surfaces and other defects, and thus introduce the complexity and diversity in the middle regime.

- (iv) **State of matter.** When the minimization of the internal energy dominates, i.e. within the A-dominated regime, the system arises as the solid state. When the maximization of entropy dominates, i.e. within the B-dominated regime, the system exists in the gaseous state. However, when the above two tendencies compromise in competition, i.e. within the A-B compromising regime, the system is at the liquid state, which might be much more complicated to describe in comparison with the solid state and the gaseous state. Since both the above two mechanisms take effects in liquid, solid-like states and gas-like states might appear in liquid alternately with respect to both space and time [16]. From this viewpoint, the criterion of minimum free energy (reflecting the compromise between two mechanisms) might not be strictly applicable to the solid or the gaseous state, though has been applied in usual practice. That is, for idealized cases where only one mechanism exists, using such a compromising criterion is not completely

reasonable. Of course, considering only one dominant mechanism is also not sufficient for non-idealized cases. Such issues should be clarified in the future.

- (v) **Gas-liquid flow.** Gas-liquid systems are similar to gas-solid fluidized systems, where the liquid phase tends to minimize its potential energy and the gas phase tends to pass the liquid phase with minimum resistance. The variational functions corresponding to these two mechanisms are gas holdup  $\varepsilon_g \rightarrow \min$  (A-dominated regime) and  $W_{st} \rightarrow \min$  (B-dominated regime), respectively. Here,  $W_{st}$  is the rate of energy consumption with respect to unit volume for suspending and transporting the liquid. Compared with that in gas-solid fluidized systems, the interphase interaction in gas-liquid systems is even more complex and regime-dependent. Under  $\varepsilon_g \rightarrow \min$ , gas bubbles and continuous liquid coexist, whereas, with  $W_{st} \rightarrow \min$ , continuous gas and liquid droplets coexist. Within the A-B compromising regime, very complex structures appear, reflecting alternate dominance of the above two mechanisms in space and time. Pre-



liminary work has been done [24], but further work is still needed to unveil this complexity.

- (vi) **Quantum mechanics and electronic systems.** Several aspects at the quantum level might also be relevant to mesoscience. (1) The uncertainty principle in quantum mechanics might originate from the coexistence of some competing mechanisms. Under the regime of local space and time with few quantum particles, different mechanisms dominate alternately, resulting in the uncertainty. With increasing scale in space and time, and hence number of quantum particles, the compromise might gradually be realized and the uncertainty gradually shrinks. From this viewpoint, the uncertainty principle might also reflect some aspects similar to the EMMS principle. (2) The ground state of an electronic system can be captured with the variational criterion of minimum energy. At other levels, however, it is found that the variational criterion is regime-specific [9,16,20]. If such a regime-specific feature of the variational criterion exists also in electronic systems, energy minimization might be the correct criterion only for one extreme regime (e.g. the A-dominated regime in Fig. 2); capturing states other than the ground state might require variational criteria for the other extreme regime (the B-dominated regime) and, of course, for the middle regime (the A-B compromising regime). Some debate at the quantum level might be from the neglect of the regime-specific feature. Therefore, if new variational criteria can be established by considering other mechanisms, e.g. dissipation mechanisms, the excited states could also be described via variational principles. (3) Wave functions, the Schrödinger equation and the density functional approach are all continuum-based, and averaging is adopted within the grid, i.e. heterogeneity within the sub-grid scale is neglected. If such heterogeneity can be included through exploiting mesoscience, the

accuracy of such models might be improved, especially for those cases where such heterogeneity is all too evident.

More issues might be of even greater interest and importance, e.g. those in neuroscience and cognitive science, life science, and strongly correlated electronic systems. Due to our limited knowledge, we will not dwell on more. Readers with relevant expertise are encouraged to do so along the above strategy.

## PERSPECTIVES AND STRATEGY TO BE FOLLOWED

The development of mesoscience calls for extensive transdisciplinary efforts [8,19], where the accumulated and abundant disciplinary knowledge from individual disciplines will be highly beneficial [17], but needs to be identified, reorganized and revisited according to the mesoscience concept, as discussed recently [9].

In addition to looking for more evidence for the EMMS principle from different fields, identifying some common rules from the study of specific problems is critical to promote mesoscience; in return, identification of common rules will greatly enable the understanding of specific problems. This two-way synergy, as practiced in our previous study, is important for the development of mesoscience. Some common rules identified and to be confirmed were discussed recently [9], including the number of dominant mechanisms, the possibility to unify the variational terms, definition of regime transitions, mathematical tools for solving multi-objective problems and the level-specific nature of mesoscale problems.

Among these issues, mathematical knowledge is critically important. A real complex system always shows dynamic behaviors resulting from the compromise in competition between dominant mechanisms formulated in different variational functions. If we solve the multi-objective variational problem directly, we will get a range of solutions corresponding to all possible states occurring in dynamic

changes. For simplification in engineering application, we usually try to look for a representative state. In this case, we need to integrate multiple variational functions (such as  $W_{st} = \min$  and  $\varepsilon = \min$ ) into a single one (such as  $N_{st} = \min$ ), which gives a fixed point of solution. How to deal with this issue and to solve the multi-objective variational problem is a challenge for mesoscience [25].

At present, mesoscience is in its infancy and its development relies fully on the interaction and cooperation between different disciplines. Every new idea usually experiences its proposition, debating and clarification, through to final verification or falsification. Only those ideas reflecting real physical laws are expected to be finally accepted, but the duration and extent of the evolution may greatly depend on the existing scientific culture. At the early stage of modern civilization, such duration was very long due to insufficient supporting knowledge and difficulty in communication. Nowadays, however, within an era of globalization and recognition of the critical importance of transdisciplinarity, the justification of the potential for mesoscience could be quite short. Therefore, no matter what is the final conclusion, we should not delay this process with habituated thinking. This is one of our purposes in writing the paper.

Understanding ‘structure’ and ‘system’ is the goal of system science [26]. As long as structure prevails in a system, no matter whether it is dynamic or stationary, we have to reveal the mechanism behind it. That is, stability condition or variational principle has to be involved. This is where we expect mesoscience to be critical. We could not guarantee the final establishment of mesoscience; however, we have sufficient confidence that exploring the concept will be a promising direction to resolve the fascinating and widespread complexity in our world.

It should be noted that the EMMS model itself is a specific formulation for gas-solid fluidization. Only the principle it follows, the principle of compromise in competition, is possibly general for all complex systems. Due to the diversity of complex systems in the whole spectrum of science and technology (shown in

Fig. 1), the formulation of each complex system must of course be developed individually though the principle of compromise in competition may be generally applicable to all complex systems. Mesoscience tries to extend this generality as much as possible, but currently the variational functions have to be identified individually.

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## REFERENCES

1. Li J, Ge W and Wang W *et al.* *From Multiscale Modeling to Meso-Science: A Chemical Engineering Perspective*. Berlin: Springer, 2013.
2. Li J and Huang W. *Towards Mesoscience: The Principle of Compromise in Competition*. Berlin: Springer, 2014.
3. Li J and Kwauk M. *Chem Eng Sci* 2003; **58**: 521–35.
4. Li J, Zhang J and Ge W *et al.* *Chem Eng Sci* 2004; **59**: 1687–1700.
5. Li J. *Chem Eng J* 2015; **278**: 541–55.
6. Li J, Huang W and Edwards PP *et al.* *arXiv* 2013; **1302**: 5861v1.
7. National Natural Science Foundation of China. 2017. <http://www.nsf.gov.cn/publish/portal0/zdyjjh/2016/info52919.htm>.
8. Li J. *Engineering* 2016; **2**: 276–85.
9. Li J, Ge W, Wang W and Yang N *et al.* *Curr Opin Chem Eng* 2016; **13**: 10–23.
10. Ge W, Chen F and Gao J *et al.* *Chem Eng Sci* 2007; **62**: 3346–77.
11. Li J. *Powder Technol* 2000; **111**: 50–9.
12. Li J, Zhang Z and Ge W *et al.* *Chem Eng Sci* 1999; **54**: 1151–4.
13. Wang L, Qiu X and Zhang L *et al.* *Chem Eng J* 2016; **300**: 83–97.
14. Huang WL and Li J. *Chem Eng Sci* 2016; **147**: 83–90.
15. Han M, Xu J and Ren Y *et al.* *Biophys Chem* 2016; **209**: 9–20.
16. Li J, Huang W and Chen J *et al.* *Chem Eng J* 2017; under review.
17. Li J, Hu Y and Yuan Q. *Sci Sin Chim* 2014; **44**: 277–81.
18. Li J, Ge W and Kwauk M. *arXiv* 2009; **0912**: 5407v4.
19. Li J. *Chem Eng J* 2015; **277**: 112–15.
20. Huang WL and Li J. *Chem Eng Sci* 2016; **155**: 233–8.
21. Xiao FS. *Personal communication*.
22. Edwards PP, Ramakrishnan TV and Rao CNR. *J Phys Chem* 1995; **99**: 5228–39.
23. Steinberg V, Voronel A and Linsky D *et al.* *Phys Rev Lett* 1980; **45**: 1338–41.
24. Yang N, Chen J and Zhao H *et al.* *Chem Eng Sci* 2007; **62**: 6978–91.
25. Li Y, Mu Y and Yuan S *et al.* *J Syst Sci Complex* 2017; **30**: 4–19.
26. Guo L. *J Syst Sci Math Sci* 2016; **36**: 291–301.

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