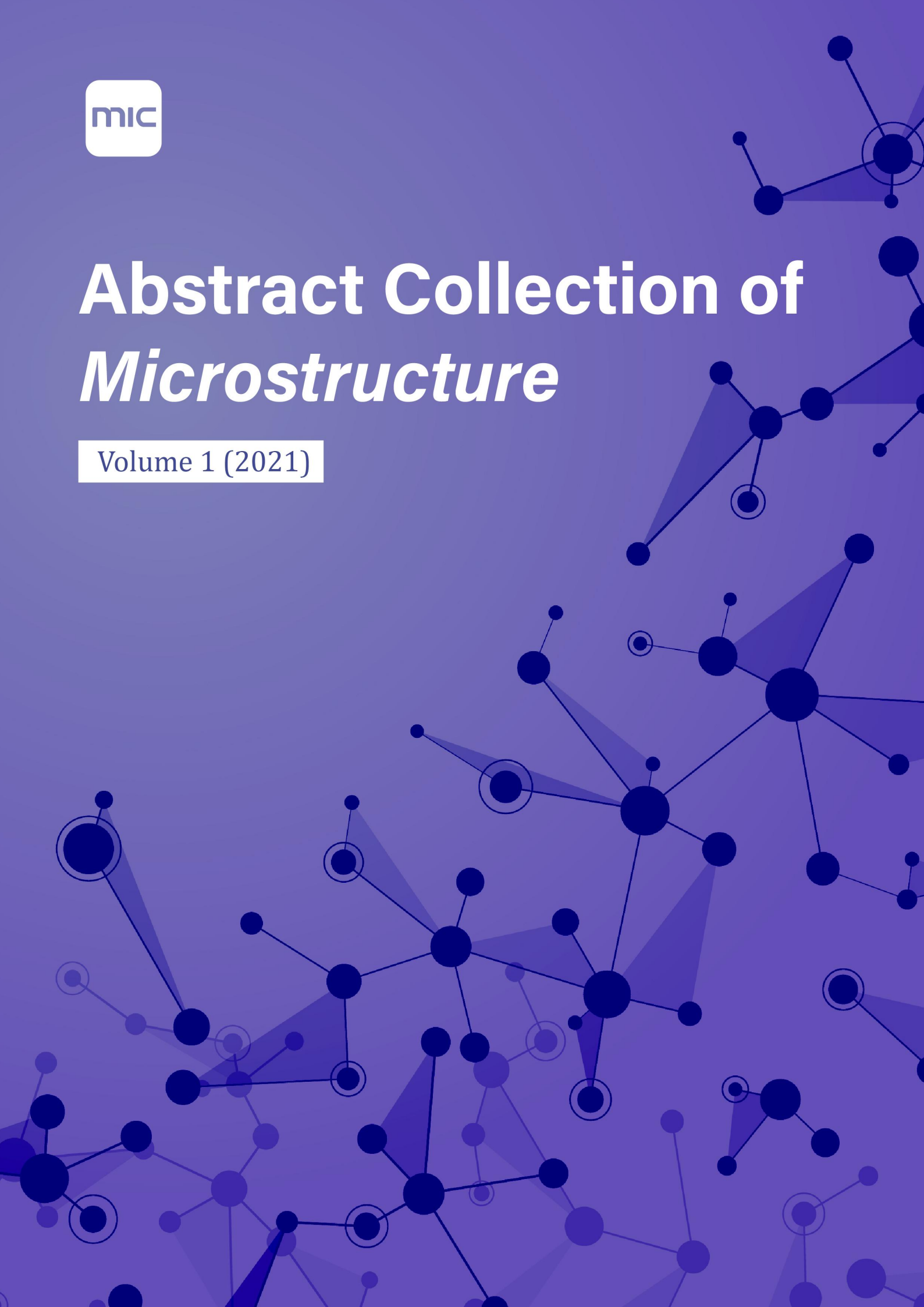




Abstract Collection of *Microstructure*

Volume 1 (2021)



Dear readers of *Microstructures*,

Here is a collection of published articles in *Microstructures* in 2021, including titles, authors, links to full paper and PDF, and citation. Abstracts and keywords are also included for those contain these parts.

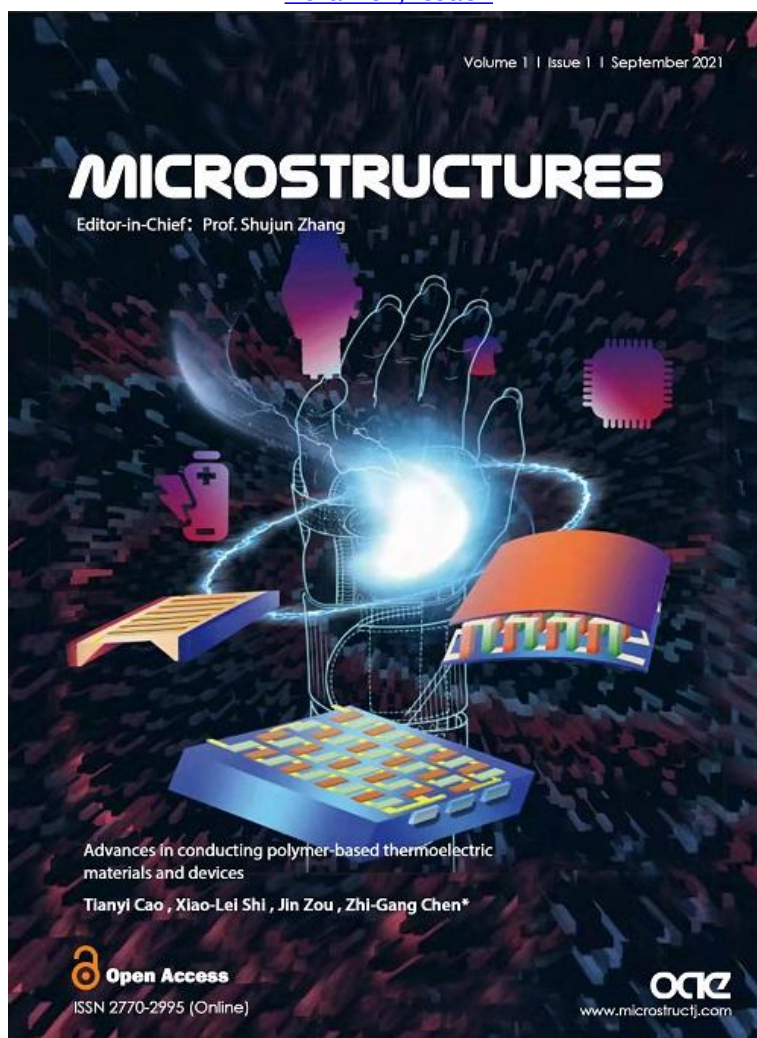
You may click the title in Contents or search keywords to locate the article quickly. We hope this collection can bring some conveniences to your reading and research. If you have any questions or suggestions on this collection, please contact us. Editorial office of *Microstructures* would be most delighted to hear from you.

Editorial Office

Microstructures

Email: editorialoffice@microstructj.com

[Volume 1, Issue 1](#)



Contents

Cover Picture	1
Advances in conducting polymer-based thermoelectric materials and devices	1
Editorial	2
The visible hand behind properties	2
Review	2
1. Thermal expansion of FeNi Invar and zinc-blende CdTe from the view point of local structure ...	2
2. EXAFS spectroscopy: a powerful tool for the study of local vibrational dynamics	3
Andrea Sanson*	3
3. Modeling-guided understanding microstructure effects in energy storage dielectrics	4
Jian Wang, Zhong-Hui Shen*	4
4. Advances in conducting polymer-based thermoelectric materials and devices	6
Research Article	7
1. Promoting the electrochemical properties of yolk-shell-structured CeO ₂ composites for lithium-ion batteries	7
2. Thermal expansion coefficient of monolayer MoS ₂ determined using temperature-dependent Raman spectroscopy combined with finite element simulations	9

Cover Picture

Advances in conducting polymer-based thermoelectric materials and devices

Tianyi Cao, Xiao-Lei Shi, Jin Zou, Zhi-Gang Chen*

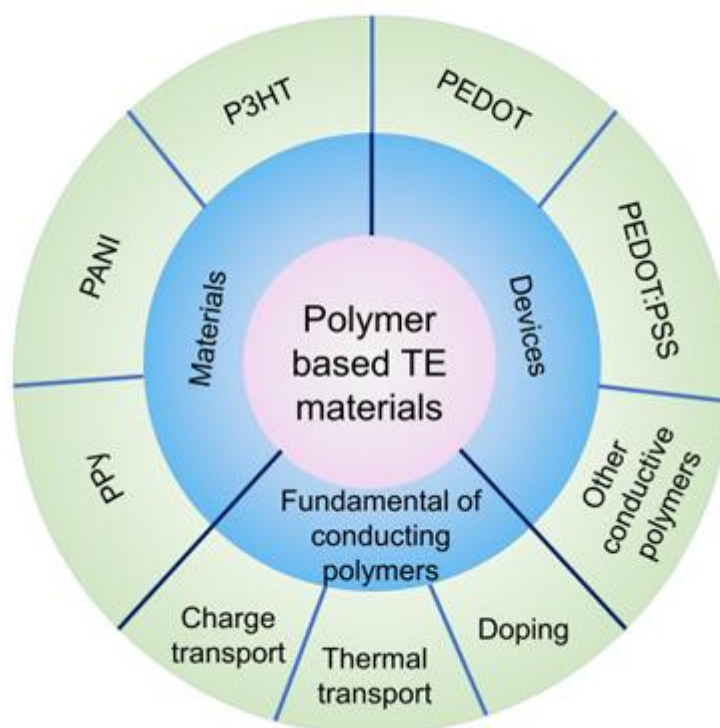
Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Graphical Abstract



Cite this article

Cao T, Shi XL, Zou J, Chen ZG. Advances in conducting polymer-based thermoelectric materials and devices. *Microstructures* 2021;1:2021007. <http://dx.doi.org/10.20517/microstructures.2021.06>

Editorial

The visible hand behind properties

Zibin Chen, Xiaozhou Liao, Jun Chen, Shujun Zhang

Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Cite this article

Chen Z, Liao X, Chen J, Zhang S. The visible hand behind properties. *Microstructures* 2021;1:2021001.

<http://dx.doi.org/10.20517/microstructures.2021.01>

Review

1. Thermal expansion of FeNi Invar and zinc-blende CdTe from the view point of local structure

Toshihiko Yokoyama*

Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Abstract

Thermal expansion of FeNi Invar and zinc-blende CdTe was investigated from the view point of local structure using the extended x-ray absorption fine structure (EXAFS) spectroscopic data and the path-integral effective classical potential (PIECP) Monte Carlo computational simulations. In this Review article, first the quantum statistical perturbation theory is intuitively described to see different character concerning thermal expansion between the quantum and classical theories. The diatomic Br₂ molecule is employed as a simple example. Second, the PIECP theory is briefly described to note advantages and disadvantages of this simulation technique. Historical background is also discussed for

the EXAFS investigation of thermal expansion based on the quantum statistical theories. The results of the FeNi Invar alloy are then summarized. The origin of zero thermal expansion in the FeNi alloy is ascribed to the so-called Invar effect that implies the variation of the electronic structure of Fe atoms depending on temperature. Zero thermal expansion at low temperature is however found to originate from the vibrational quantum effect. It is also noted that the interatomic distances of Fe-Fe, Fe-Ni, and Ni-Ni pairs are slightly but meaningfully different from each other, although the alloy exhibit a simple fcc crystal. Such a pair-dependent difference is also true for thermal expansion and we will discuss thermal expansion from the local point of view, which is interestingly different from the lattice thermal expansion significantly. Finally, the results of the zinc blende (or diamond) structure are presented. Although the origin of negative thermal expansion in these tetrahedral crystals is known as a result of classical vibrational anomaly within the Newton dynamics theory, the quantum statistical simulation is found to be essential to reproduce the negative thermal expansion of CdTe. It is emphasized that the vibrational quantum effect and classical anharmonicity are of great importance for the understanding of low-temperature thermal expansion as well as the elastic constants.

Keywords

Thermal expansion, Invar alloy, zinc blende, EXAFS, Monte Carlo simulation, path integral effective classical potential method

Cite this article

Yokoyama T. Thermal expansion of FeNi Invar and zinc-blende CdTe from the view point of local structure. *Microstructures* 2021;1:2021003. <http://dx.doi.org/10.20517/microstructures.2021.001>

2. EXAFS spectroscopy: a powerful tool for the study of local vibrational dynamics

Andrea Sanson*

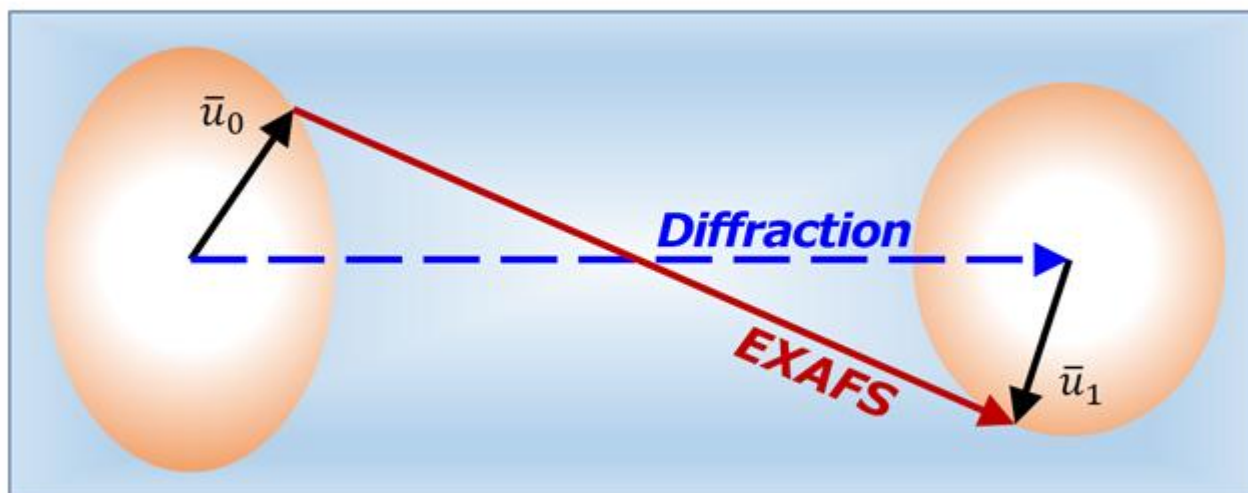
Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Graphical Abstract



Abstract

Extended X-ray absorption fine structure (EXAFS) spectroscopy is an ideal technique for studying the local vibrational dynamics of materials due to its sensitivity to short-range order, correlation of atomic motion and anharmonicity. However, despite this, EXAFS is widely employed to investigate the local structure but its use in the study of local dynamics is far more limited. In this brief review, the potential of EXAFS as a vibrational probe is presented with the aim of promoting its application in the study of the local dynamics of solid-state materials.

Keywords

EXAFS, local dynamics, thermal disorder

Cite this article

Sanson A. EXAFS spectroscopy: a powerful tool for the study of local vibrational dynamics.

Microstructures 2021;1:2021004. <http://dx.doi.org/10.20517/microstructures.2021.03>

3. Modeling-guided understanding microstructure effects in energy storage dielectrics

Jian Wang, Zhong-Hui Shen*

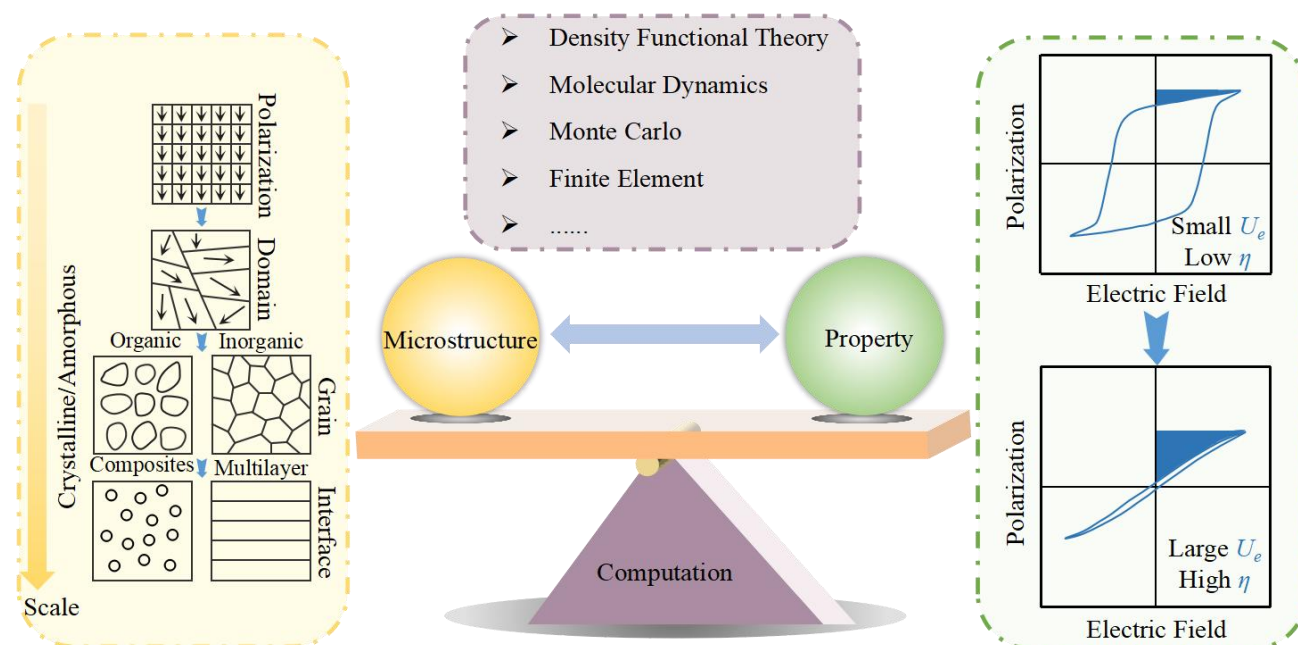
Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Graphical Abstract



Abstract

Addressing the relationships between microstructures and properties is critical to the design of novel dielectric capacitors, which further enables widespread promising applications in electronic and electrical systems. The present review focuses on the role of different theoretical modeling techniques in understanding microstructural effects in energy storage dielectrics. State-of-the-art developments in the computational modeling of inorganics, polymers and their composite dielectrics are summarized. Diverse microstructural effects, including domain configurations, crystallization behavior and composite structures, are discussed with regards to different models. Theoretical modeling is not only essential for gaining fundamental insights into the underlying mechanisms behind experimental phenomena but can also be used to inversely engineer the design of dielectrics by prediction or optimization. Finally, to further promote innovative developments in dielectric capacitors, some future perspectives are provided to stimulate the in-depth consideration of the research paradigm between modeling and experiment.

Keywords

Theoretical modeling, microstructural effects, energy storage, dielectric capacitors

Cite this article

Wang J, Shen ZH. Modeling-guided understanding microstructure effects in energy storage dielectrics.

Microstructures 2021;1:2021006. <http://dx.doi.org/10.20517/microstructures.2021.05>

4. Advances in conducting polymer-based thermoelectric materials and devices

Tianyi Cao, Xiao-Lei Shi, Jin Zou, Zhi-Gang Chen*

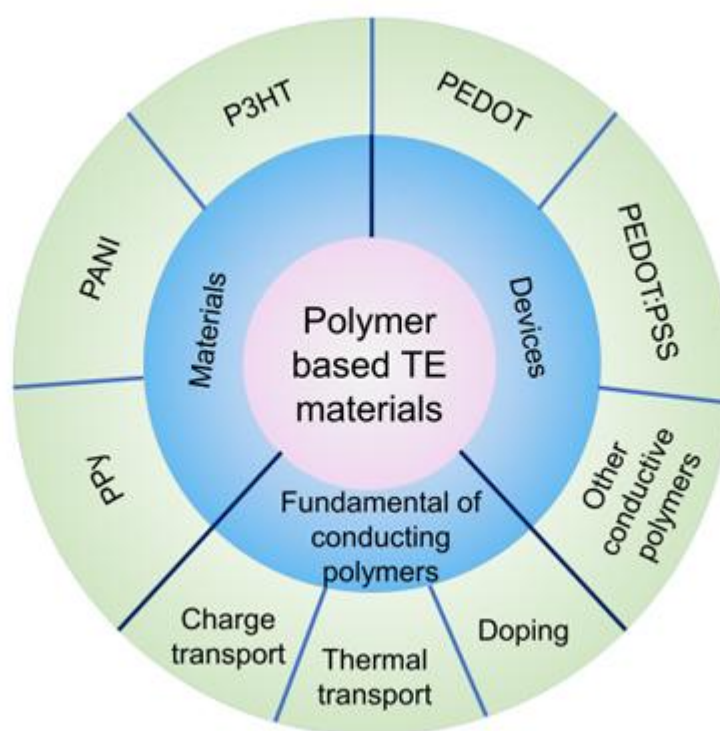
Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Graphical Abstract



Abstract

Conducting polymer-based thermoelectric materials are considered the most promising candidates for applying to wearable thermoelectric devices because of their high electrical conductivities, flexibility, stability, and low-toxicity features. Therefore, a timely review is needed to comprehensively overview their most recent progress in the last few years, considering the rapid development of thermoelectric conducting polymers. In this work, we carefully summarize recent advances in thermoelectric

conducting polymers from aspects of their mechanisms, synthesis, micro/nanostructures, mechanical/thermoelectric properties, and related functional devices. A few state-of-the-art thermoelectric conducting polymers, including poly(3,4-ethylenedioxythiophene)poly(styrenesulfonate), poly(3-hexylthiophene), polyaniline, and polypyrrole, are highlighted in detail. In the end, we point out the challenges, controversies, and outlooks of conducting polymers for future thermoelectric applications.

Keywords

Thermoelectric, conducting polymer, synthesis, performance, device

Cite this article

Cao T, Shi XL, Zou J, Chen ZG. Advances in conducting polymer-based thermoelectric materials and devices. *Microstructures* 2021;1:2021007. <http://dx.doi.org/10.20517/microstructures.2021.06>

Research Article

1. Promoting the electrochemical properties of yolk-shell-structured CeO₂ composites for lithium-ion batteries

Yongchao Shi, Jipeng Fu*, Kanglong Hui, Jie Liu, Cong Gao, Shuqin Chang, Yongjin Chen, Xiang Gao, Tian Gao, Ligang Xu, Qi Wei, Mingxue Tang*

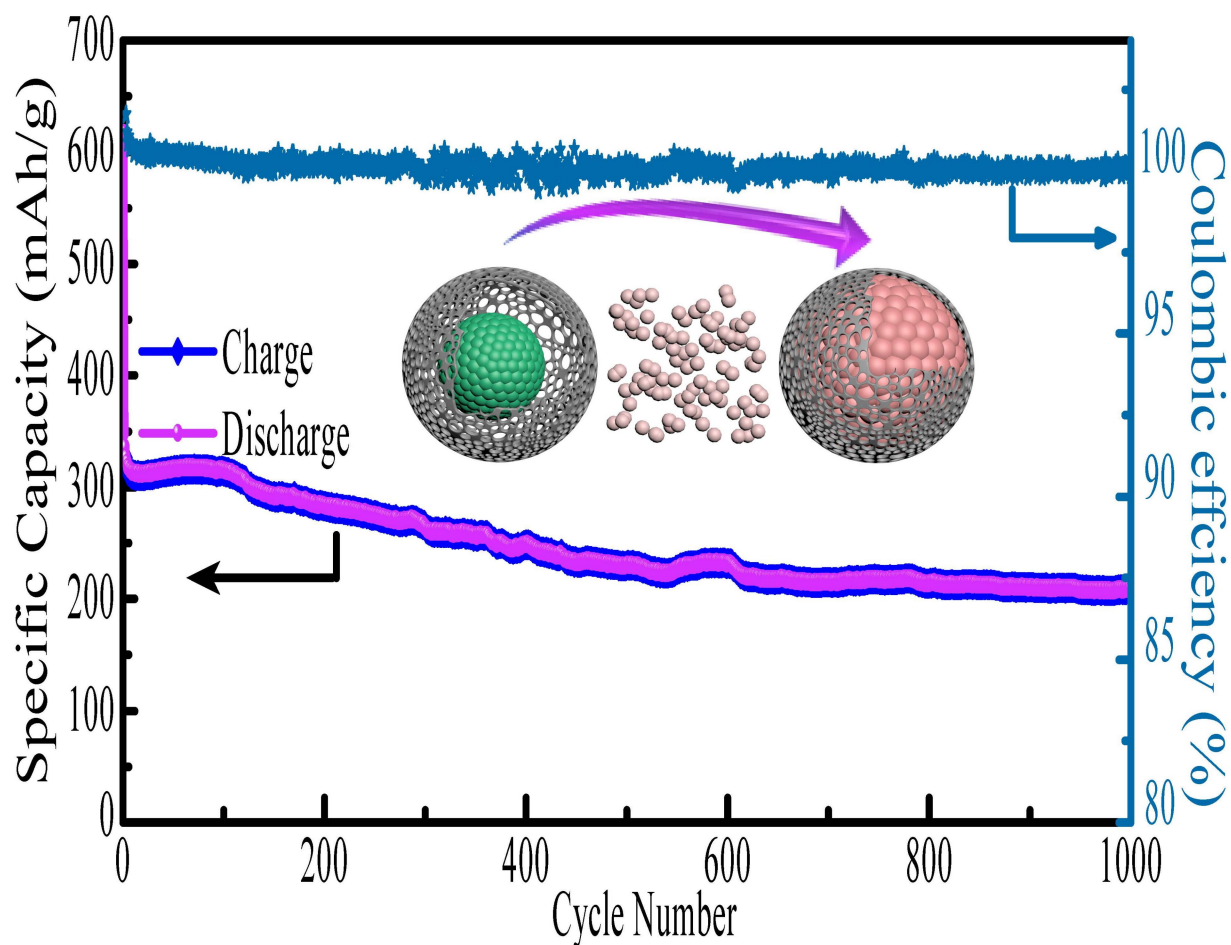
Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Graphical Abstract



Abstract

Lithium-ion batteries offer significant convenience to modern portable technology and our daily lives due to their high energy density and cycling capabilities. Cerium oxides are attracting significant attention as Li-ion battery anode materials due to their nontoxicity and fast redox kinetics. However, these anodes face critical issues, such as poor electronic conductivity and serve volume expansion upon Li-ion intercalation. Herein, yolk-shell-structured CeO_2 encapsulated in mesoporous carbon nanospheres ($\text{CeO}_2@\text{void}@\text{C}$) is proposed with an adjustable void between the CeO_2 core and the outer carbon layer. A significantly enhanced capacity and rate performance are obtained for the target $\text{CeO}_2@\text{void}@\text{C}$ when compared with the untreated CeO_2 anode. The reversible capacity of $\text{CeO}_2@\text{void}@\text{C}$ is double that of the untreated CeO_2 anode. Additionally, the yolk-shell-structured CeO_2 shows a slow capacity decay and maintains a capacity of $210 \text{ mAh}\cdot\text{g}^{-1}$ at a current density of $1000 \text{ mA}\cdot\text{g}^{-1}$ with a $\sim 100\%$ Coulombic efficiency even after 1000 cycles. This improvement originates from the conductivity of the coating carbon layer and the void that constrains the volume change upon electrochemical lithiation/delithiation.

Keywords

Li-ion batteries, microstructures, volume constraints, yolk-shell structures, anode materials, CeO₂ composites

Cite this article

Shi Y, Fu J, Hui K, Liu J, Gao C, Chang S, Chen Y, Gao X, Gao T, Xu L, Wei Q, Tang M. Promoting the electrochemical properties of yolk-shell-structured CeO₂ composites for lithium-ion batteries.

Microstructures 2021;1:2021005. <http://dx.doi.org/10.20517/microstructures.2021.04>

2. Thermal expansion coefficient of monolayer MoS₂ determined using temperature-dependent Raman spectroscopy combined with finite element simulations

Yang Yang, Zhongtao Lin, Renfei Li, Yutong Li, Wuguo Liu, Shibing Tian, Ke Zhu, Lianchun Long*

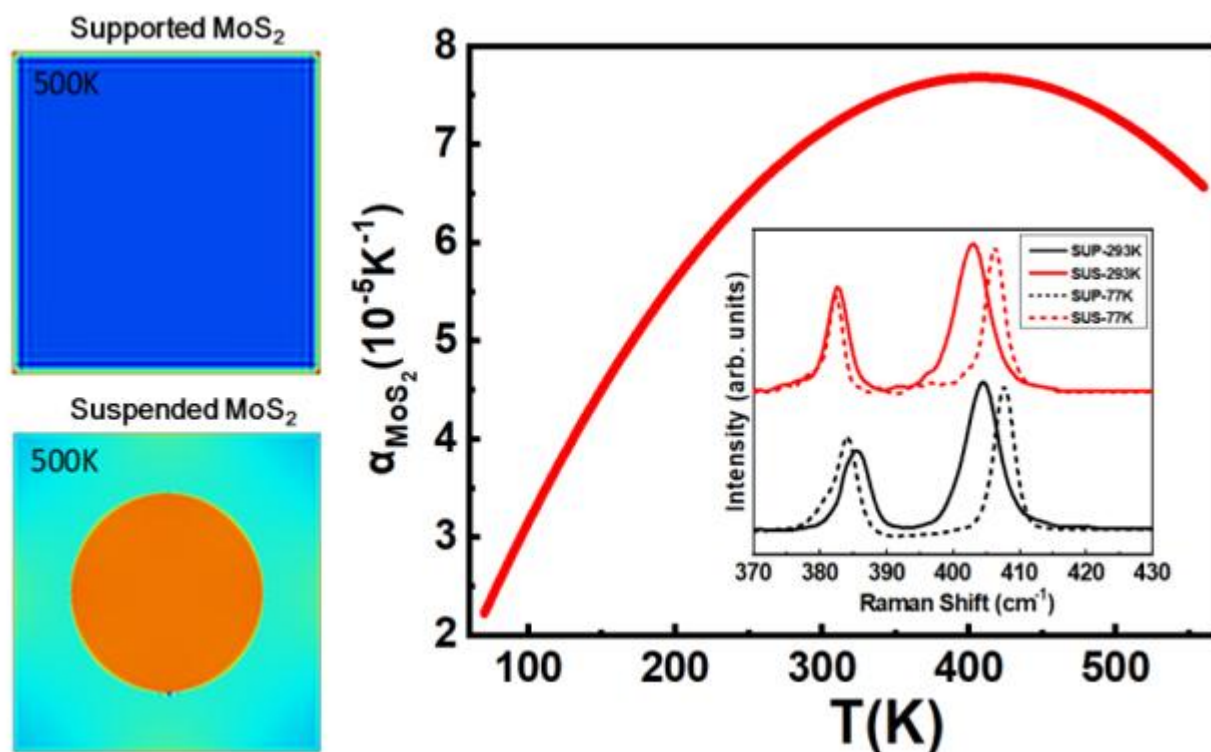
Read

[Full-text](#) [PDF](#)

Citation

[RIS](#)

Graphical Abstract



Abstract

The thermal expansion coefficient is an important parameter of monolayer MoS₂ that affects the performance of its related optoelectronic devices. To obtain the thermal expansion coefficient of monolayer MoS₂, suspended and supported MoS₂ are systematically investigated using micro-Raman spectroscopy in a temperature range of 77-557 K. Obvious differences in the temperature-dependent evolution of the Raman peaks between suspended and supported MoS₂ are observed, which result from the thermal expansion coefficient mismatch between MoS₂ and the substrate. With the help of the finite element method, the thermal strain in suspended and supported MoS₂ is calculated and used to deduce the thermal expansion coefficient mismatch-induced Raman shift. By matching the simulation and experimental results, the thermal expansion coefficient of MoS₂ is identified through the numerical inversion calculation. Our results demonstrate that the combination of micro-Raman spectroscopy and finite element simulations is highly effective for identifying the intrinsic thermal expansion coefficient of two-dimensional materials.

Keywords

Monolayer MoS₂, thermal expansion coefficient, Raman spectroscopy, finite element method

Cite this article

Yang Y, Lin Z, Li R, Li Y, Liu W, Tian S, Zhu K, Long L. Thermal expansion coefficient of monolayer MoS₂ determined using temperature-dependent Raman spectroscopy combined with finite element simulations. *Microstructures* 2021;1:2021002. <http://dx.doi.org/10.20517/microstructures.2021.02>