443.
标题: Enhanced Thermal Diffusion of Li in Graphite by Alternating Vertical Electric Field: A Hybrid Quantum-Classical Simulation Study
作者: Ohba, N (Ohba, Nobuko); Ogata, S (Ogata, Shuji); Tamura, T (Tamura, Tomoyuki); Kobayashi, R (Kobayashi, Ryo); Yamakawa, S (Yamakawa, Shunsuke); Asahi, R (Asahi, Ryoji)
来源出版物: JOURNAL OF THE PHYSICAL SOCIETY OF JAPAN 卷: 81 期: 2 文献号: 023601 DOI: 10.1143/JPSJ.81.023601 出版年: FEB 2012

引用的参考文献数: 24
摘要: Enhancing the diffusivity of the Li ion in a Li-graphite intercalation compound that has been used as a negative electrode in the Li-ion rechargeable battery, is important in improving both the recharging speed and power of the battery. In the compound, the Li ion creates a long-range stress field around itself by expanding the interlayer spacing of graphite. We advance the hybrid quantum-classical simulation code to include the external electric field in addition to the long-range stress field by first-principles simulation. In the hybrid code, the quantum region selected adaptively around the Li ion is treated using the real-space density-functional theory for electrons. The rest of the system is described with an empirical interatomic potential that includes the term relating to the dispersion force between the C atoms in different layers. Hybrid simulation runs for Li dynamics in graphite are performed at 423 K under various settings of the amplitude and frequency of alternating electric fields perpendicular to C-layers. We find that the in-plane diffusivity of the Li ion is enhanced significantly by the electric field if the amplitude is larger than 0.2 V/angstrom within its order and the frequency is as high as 1.7 THz. The microscopic mechanisms of the enhancement are explained.
入藏号: WOS:000299822100002
语种: English
文献类型: Article
作者关键词: Li-graphite intercalation compound; electric field; hybrid simulation; density functional theory; Li diffusion
KeyWords Plus: PYROLYTIC-GRAPHITE; PARALLEL COMPUTERS; LITHIUM
地址: [Ohba, Nobuko; Yamakawa, Shunsuke; Asahi, Ryoji] Toyota Cent Res & Dev Labs Inc, Nagakute, Aichi 4801192, Japan
[Ohba, Nobuko; Ogata, Shuji; Tamura, Tomoyuki; Kobayashi, Ryo] Nagoya Inst Technol, Grad Sch Engn, Nagoya, Aichi 4668555, Japan
通讯作者地址: Ohba, N (通讯作者),Toyota Cent Res & Dev Labs Inc, Nagakute, Aichi 4801192, Japan
出版商: PHYSICAL SOC JAPAN
出版商地址: EISHIN-KAIHATSU BLDG, 5TH FLR, 5-34-3 SHINBASHI, MINATO-KU, TOKYO 105-0004, JAPAN
Web of Science 分类: Physics, Multidisciplinary
学科类别: Physics
IDS 号: 886AH
ISSN: 0031-9015
29 字符的来源出版物名称缩写: J PHYS SOC JPN

ISO 来源出版物缩写: J. Phys. Soc. Jpn.
来源出版物页码计数: 4