材料研究にICSDを利用した研究論文リスト

2019.11 化学情報協会 調べ

1. Effect of crystal structure on CO_2 capture characteristics of dry potassium-based sorbents.
   Chuanwen Zhao, Xiaoping, Chen, Changsui Zhao, *Chemosphere*, 75, 10, 2009, 1401-1404.
   https://doi.org/10.1016/j.chemosphere.2009.02.045
   カリウムベース吸着剤のCO_2吸着について.

2. Design Strategy for High-Performance Thermoelectric Materials: The Prediction of Electron-Doped $KZrCuSe_3$
   Shiqiang Hao, Logan Ward, Zhongzhen Luo, Vidvuds Ozolins, Vinayak P. Dravid, Mercouri G. Kanatzidis, and Christopher Wolverton. *Chem. Mater.* **2019**, 31, 8, 3018–3024.
   https://doi.org/10.1021/acs.chemmater.9b00840
   性能指数の高い熱電材料を特定するための効率的な戦略.

3. Candidate Inorganic Photovoltaic Materials from Electronic Structure-Based Optical Absorption and Charge Transport Proxies
   Douglas H. Fabini, Mitchell Koerner, and Ram Seshadri. *Chem. Mater.* **2019**, 31, 5, 1561–1574.
   https://doi.org/10.1021/acs.chemmater.8b04542
   光起電（PV）吸収体の探索.

4. Combined Theoretical Approach for Identifying Battery Materials: Alsup3+ Mobility in Oxides
   Tina Nestler, Falk Meutzner, Artem A. Kabanov, Matthias Zschornak, Tilmann Leisegang, and Dirk Carl Meyer. *Chem. Mater.* **2019**, 31, 3, 737–747. https://doi.org/10.1021/acs.chemmater.8b03631
   Al イオン電池の材料.

5. Sulfur- and Selenium-Containing Compounds Potentially Exhibiting Al Ion Conductivity.
   Meutzner F., Zschornak M.,Kabanov A. A., Nestler T. ,Leisegang T., Blatov V. A., Meyer D. C., *Chemistry*, **2019**, 25(36), 8623-8629. https://doi.org/10.1002/chem.201901438
   Alのイオン電導に関する研究.

6. Computational Screening of Hydration Reactions for Thermal Energy Storage: New Materials and Design Rules
   Steven Kiyabu, Jeffrey S. Lowe, Alauddin Ahmed, and Donald J. Siegel. *Chem. Mater.* **2018**, 30, 6, 2006–2017. https://doi.org/10.1021/acs.chemmater.7b05230
   熱エネルギー貯蔵（TES）材料.

7. High-throughput search for potential potassium ion conductors: A combination of geometrical-topological and density functional theory approaches
   R. A. Eremin, N. A. Kabanova, Ye. A. Morkhova, A. A. Golov, V. A. Blatov. *Solid state ionics*, 2018, 326, 188-199. https://doi.org/10.1016/j.ssi.2018.10.009
   カリウム固体電解質．高速幾何学的トポロジーアプローチと正確な DFT モデリングの組み合わせで、結晶性固体のイオン伝導率の予測.

8. Identification of a narrow band red light-emitting phosphor using computational screening of ICSD: Its synthesis and optical characterization
   Minseuk Kim, Satendra Pal Singha, Jin-Woong Lee, Takamasa Izawa, Dohoon Kim, Bonggoo Yun, chulsoo Yoon, Woon Bae Park, Kee-Sun Sohn. *Journal of Alloys and Compounds*, **2019**, 774, 5, 338-346.
   https://doi.org/10.1016/j.jallcom.2018.09.370

ICSDから赤色蛍光体発光ダイオード（LED）の候補を検索.

9. Crystallochemical tools in the search for cathode materials of rechargeable Na-ion batteries and analysis of their transport properties
Stanislav S. Fedotov, Natalya A. Kabanova, Artem A. Kabanov, Vladislav A. Blatov, Nellie R. Khasanova, Evgeny V. Antipo. *Solid State Ionics*, 314, **2018**, 129-140. https://doi.org/10.1016/j.ssi.2018.10.009
Naイオン電池のカソード材料.

10. Computational investigation of inverse-Heusler compounds for spintronics applications
Jianhua Ma, Jiangang He, Dipanjan Mazumdar, Kamaram Munira, Sahar Keshavarz, Tim Lovorn, C. Wolverton, Avik W. Ghosh, and William H. Butler. *Phys. Rev. B*, 98, 094410 (2018).
https://doi.org/10.1103/PhysRevB.98.094410
逆ホイスラー化合物のスピントロニクス材料. 理論計算と ICSD の実際の構造との比較.

11. Screening for Cu-S based thermoelectric materials using crystal structure features
Rui-zhi Zhang, Kan Chen, Baoli Du, and Michael J. Reece. *J. Mater. Chem. A*, **2017**, 5, 5013-5019.
https://doi.org/10.1039/C6TA10607B
Cu–Sベースの熱電材料化合物. ICSDからハイスループットスクリーニングで候補を特定.

12. Prediction of new stable structure, promising electronic and thermodynamic properties of MoS_3: Ab initio calculations
Yong Pan, Weiming Guan. *Journal of Power Sources*, 325, **2016**, 246-251.
https://doi.org/10.1016/j.jpowsour.2016.06.044
水素貯蔵材料の MoS_3 の構造，関連する物理的および熱力学的特性を体系的に調査.

13. Computational and experimental investigation for new transition metal selenides and sulfides: the importance of experimental verification for stability
Awadhesh Narayan, Ankita Bhutani, Samantha Rubeck, James N. Eckstein, Daniel P. Shoemaker, and Lucas K. Wagner. *Phys. Rev. B*, 94, 045105 (2016). https://doi.org/10.1103/PhysRevB.94.045105
相関電子特性を持つセレンや硫黄などの遷移金属カルコゲニドの探索.

14. Novel high-K dielectrics for next-generation electronic devices screened by automated ab initio calculations
Kanghoon Yim, Youn Yong, Joohee Lee, Kyuhyun Lee, Ho-Hyun Nahm, Jiho Yoo, Chanhee Lee, Cheol Seong Hwang & Seungwu Han. *NPG Asia Materials*, 7, e190 (2015). https://doi.org/10.1038/am.2015.57
より大きな誘電率とバンドギャップを示す high-κ 材料

15. Screening of the alkali-metal ion containing materials from the Inorganic Crystal Structure Database (ICSD) for high ionic conductivity pathways using the bond valence method
Max Avdeev, Matthew Sale, Stefan Adams, R. Prasada Rao. *Solid State Ionics*, 225, 4, **2012**, 43-46.
https://doi.org/10.1016/j.ssi.2012.02.014
高イオン伝導率を持つ電解質や電極材料開発のためのスクリーニング.

16. Multivariate method-assisted ab initio study of olivine-type $LiMXO_4$ (main group M^{2+}-X^{5+} and M^{3+}-X^{4+}) compositions as potential solid Electrolytes
Randy Jalem, Takahiro Aoyama, Masanobu Nakayama, and Masayuki Nogami. *ChemInform*, 24(7):1357–1364 (2012). https://doi.org/10.1021/cm3000427
高性能の全固体充電式リチウムイオン電池の開発のためのリチウムイオン伝導性固体酸化物電解質の検索.