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SCI Papers

1. Jia Zhang, Lei Kang, Tse-Hsing Lin, Xingxing Jiang, Pifu Gong, **Ming-Hsien Lee*** and Zheshuai Lin* (2015, Nov). The mechanism for the nonlinear optical properties in La₉Na₃B₈O₂₇, La₂Na₃B₃O₉ and La₂CaB₁₀O₁₉: ab initio studies. *Journal of Physics: Condensed Matter*, 27, 485501. (SCI, 20/67, Physics, Condensed Matter). 本人為通訊作者.
2. Weiwei Ji, **Ming-Hsien Lee**, Luyuan Hao, Xin Xu*, Simeon Agathopoulos, Dewen Zheng, and Chaohe Fang (2015, Feb). Role of Oxygen Vacancy on the Photoluminescence of BaMgSiO₄:Eu Phosphors: Experimental and Theoretical Analysis. *Inorganic Chemistry*, 54, 1556-1562. (SCI, 4/45, Chemistry Inorganic and Nuclear).
3. Bingbing Zhang, **Ming-Hsien Lee**, Zhihua Yang*, Qun Jing, Shilie Pan*, Min Zhang, Hongping Wu, Xin Su, and Cheng-Shun Li (2015, Jan). Simulated pressure-induced blue-shift of phase-matching region and nonlinear optical mechanism for K₃B₆O₁₀X (X=Cl, Br). *Applied Physics Letters*, 106, 031906. (SCI, 21/144, Physics, Applied).
4. Li-Cheng Ju, Xin Xu, Lu-Yuan Hao, Yue Lin, **Ming-Hsien Lee** (2015, Jan). Modification of the coordination environment of Eu²⁺ in Sr₂SiO₄:Eu²⁺ phosphors to achieve full color emission. *Journal of Materials Chemistry C*, 3(7):1567-1575. (SCI, 18/144, Physics, Applied).
5. Xin Su, Zhihua Yang, **Ming-Hsien Lee**, Shilie Pan, Ying Wang, Xiaoyun Fan, Zhenjun Huang, Bingbing Zhang (2015, Jan). Evidence of “new hot spots” from determining the nonlinear optical behavior of materials: mechanistic studies of the vanadium borate crystal, Na₃VO₂B₆O₁₁. *Physical Chemistry Chemical Physics*, 17(7), 5338. (SCI, 6/34, physics, atomic, molecular and chemical).
6. **Ming-Hsien Lee**; Yen-Chun Peng; Hsuan-Chung Wu* (2014, Dec). Effects of intrinsic defects on electronic structure and optical properties of Ga-doped ZnO. *Journal of Alloys and Compounds*, 616, p.122–127. (SCI, 5/75, METALLURGY& METALLURGICAL ENGINEERING). 本人為第一作者.
7. Xingxing Jiang; Lei Kang; Siyang Luo; Pifu Gong; **Ming-Hsien Lee***; Zheshuai Lin* (2014, Nov). Development of nonlinear optical materials promoted by density functional theory simulations. *International Journal of Modern Physics B*, Vol. 28, 1430018. (SCI, 60/67, PHYSICS CONDENSED MATTER). 本人為通訊作者.
8. Chen Lei; Zhihua Yang*; Bingbing Zhang; **Minghsien Lee**; Qun Jing; Zhaohui Chen; Xuchu Huang; Ying Wang; Shilie Pan*; Muhammad Ramzan Saeed Ashraf Janjua (2014, Aug). The Influence of Hydrogen Bonding on the Nonlinear Optical Properties of a Semiorganic Material

NH₄B[D-(+)]C₄H₄O₅]·2 H₂O: A Theoretical Perspective. *Phys. Chem. Chem. Phys.*, 16(37):20089-96. (SCI, 5/33, PHYSICS, ATOMIC, MOLECULAR & CHEMICAL).

9. Lin Hao; Lei Yang; **Ming-Hsien Lee**; Tseh-Hsing Lin; ZhongFeng Zhang; XiangNan Xie; Hong Zhu* (2014, Jul). Layered B-site cation ordering: A key factor in ferrimagnetism of Y₂MnCrO₆. *Journal of Alloys and Compounds*, 601, 14 - 18 . (SCI, 5/75, METALLURGY & METALLURGICAL ENGINEERING).
10. Zheshuai Lin*; Xingxing Jiang; Lei Kang; Pifu Gong; Siyang Luo; **Ming-Hsien Lee** (2014, Jun). First-principles materials applications and design of nonlinear optical crystals. *Journal of Physics D Applied Physics*, 47, 253001. (SCI).
11. Bingbing Zhang; Zhihua Yang*; Yun Yang; **Ming-Hsien Lee**; Shilie Pan*; Qun Jin; Xin Su (2014, Apr). p-(p, pi*) interaction mechanism revealing and accordingly designed new member in deep-ultraviolet NLO borates LinMn₁B_{2n-1}O_{4n-2} (M=Cs/Rb, n=3, 4, 6). *Journal of Materials Chemistry C*, Vol. 2, Issue 21, p.4133-4141. (SCI).
12. Jia-Ye Tang , Jing-Kun Gao , Jun-Hua Chen , Lu-Yuan Hao , Xin Xu , **MingHsien Lee** (2013, Jul). Contribution of cations to the photoluminescence properties of Eu-doped barium oxonitridosilicates phosphors. *Computational Materials Science*, Vol.79 (06), pp.478-484. (SCI, 81/251, MATERIALS SCIENCE, MULTIDISCIPLINARY).
13. Xin Su, Ying Wang, Zhihua Yang, Xu-Chu Huang, Shilie Pan, Feng Li, and **Ming-Hsien Lee** (2013, Jun). Experimental and Theoretical Studies on the Linear and Nonlinear Optical Properties of Bi₂ZnOB₂O₆. *Journal of Physical Chemistry C*, 117, 14149. (SCI, 29/251, MATERIALS SCIENCE, MULTIDISCIPLINARY).
14. **Ming-Hsien Lee**, Po-Liang Liu, Yung-An Hong, Yen-Ting Chou, Jia-Yang Hong, and Yu-Jin Siao (2013, Feb). Electronic band structures of Ge_{1-x}Sn_x semiconductors: A first-principles density functional theory study. *Journal of Applied Physics*, 113, 063517. (SCI, 39/136 PHYSICS, APPLIED). 本人為第一作者.
15. Zhihua Yang, Shilie Pan, Hongwei Yu, **Ming-Hsien Lee** (2013, Jan). Electronic structure and optical properties of the nonlinear optical crystal Pb₄O(BO₃)₂ by first-principles calculations. *Journal of Solid State Chemistry*, 198, 77–80. (SCI, 16/45, CHEMISTRY, INORGANIC & NUCLEAR).
16. Yi-fei Wang, Jing-kun Gao, **Ming-Hsien Lee**, Wei He, Xin Xu, Lu-yuan Hao, and Jun-hua Chen (2012, Aug). First-principle Studies on Enhanced Optical Stability of BaMgAl₁₀O₁₇:Eu²⁺ Phosphor by SiN Doping. *Chinese Journal of Chemical Physics*, 25, 398. (SCI, 31/33, PHYSICS, ATOMIC, MOLECULAR & CHEMICAL).
17. Liang-Jun Yin, Qiang-Qiang Zhu, Wei Yu, Lu-Yuan Hao, Xin Xu, Feng-Chun Hu, and **Ming-Hsien Lee** (2012, Mar). Europium location in the AlN: Eu green phosphor prepared by a gas-

reduction-nitridation route. *Journal of Applied Physics*, 111, 053534. (SCI, 39/136, PHYSICS, APPLIED).

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