

Bibliography

- [1] Malathi Arumugam, Muhammad Tahir, and Piyasan Prasertthdam. *Chemosphere*, 286:131765, 2022.
- [2] Mike C. Payne, Michael P. Teter, Douglas C. Allan, Tomás Arias, and J. D. Joannopoulos. *Rev. Mod. Phys.*, 64:1045–1097, 1992.
- [3] Xiaofan Yang, Xiaoming Liu, Shuo Yu, Lu Gan, Jun Zhou, and Yonghu Zeng. *Electronics*, 8(8), 2019.
- [4] Graeme Henkelman, Blas P. Uberuaga, and Hannes Jónsson. *Chem. Phys.*, 113(22):9901–9904, 2000.
- [5] Graeme Henkelman and Hannes Jónsson. *Chem. Phys.*, 111(15):7010–7022, 1999.
- [6] Jinshui Zhang, Xiufang Chen, Kazuhiro Takanabe, Kazuhiko Maeda, Kazunari Domen, JanDirk Epping, Xianzhi Fu, Markus Antonietti, and Xinchun Wang. *Angew. Chem., Int. Ed. Engl.*, 49(2):441–444, 2010.
- [7] Nirmala Thorat, Asha Yadav, Manisha Yadav, Suraj Gupta, Ranjana Varma, Saju Pillai, Rohan Fernandes, Maulik Patel, and Nainesh Patel. *J. Environ. Manage.*, 247:57–66, 2019.
- [8] Brajesh R. Bhagat and Alpa Dashora. *Carbon*, 178:666–677, 2021.
- [9] Brajesh R. Bhagat, Kishan H. Mali, and Alpa Dashora. *J. Phys. Chem. C*, 126(5):2573–2586, 2022.

- [10] Omid Akhavan and Elham Ghaderi. *Surf. Coat. Technol.*, 204(21):3676–3683, 2010.
- [11] Hyun Soo Lee, Se Joon Im, Jong Hak Kim, Hee Jin Kim, Jong Pyo Kim, and Byoung Ryul Min. *Desalination*, 219(1):48–56, 2008.
- [12] Gongming Wang, Yichuan Ling, Hanyu Wang, Xunyu Yang, Changchun Wang, Jin Z. Zhang, and Yat Li. *Energy Environ. Sci.*, 5:6180–6187, 2012.
- [13] Dagui Chen, Feng Huang, Guoqiang Ren, Dongsong Li, Meng Zheng, Yongjing Wang, and Zhang Lin. *Nanoscale*, 2:2062–2064, 2010.
- [14] Chungui Tian, Qi Zhang, Aiping Wu, Meijia Jiang, Zhenglan Liang, Baojiang Jiang, and Honggang Fu. *Chem. Commun.*, 48:2858–2860, 2012.
- [15] Lei Cheng, Quanjun Xiang, Yulong Liao, and Huaiwu Zhang. *Energy Environ. Sci.*, 11:1362–1391, 2018.
- [16] Gowhar A. Naikoo, H. Salim, T. Awan, Israr U. Hassan, Musallam A. Tabook, Mona Z. Pedram, M. Mustaqeem, and T.A. Saleh. *Mater. Today Chem.*, 26:101108, 2022.
- [17] J Mater Sci Technol . 56:18–44, 2020.
- [18] Shagufta Riaz, Munir Ashraf, Tanveer Hussain, Muhammad Tahir Hussain, and Ayesha Younus. *Colloids Surf. A Physicochem. Eng. Asp.*, 581:123799, 2019.
- [19] Y Ma, C P Wong, X T Zeng, T Yu, Y Zhu, and Z X Shen. *J. Phys. D*, 42(6):065417, 2009.
- [20] Justus Liebig. *Ann. Phar.*, 10(1):1–47, 1834.
- [21] Amy Y. Liu and Marvin L. Cohen. *Science*, 245(4920):841–842, 1989.
- [22] Bicheng Zhu, Liuyang Zhang, Bei Cheng, and Jiaguo Yu. *Appl. Catal. B Environ*, 224:983–999, 2018.

-
- [23] Waseem Raza, D. Bahnemann, and M. Muneer. *J. Photochem. Photobiol. A*, 342:102–115, 2017.
- [24] S. Lu, Zhiwen W. Chen, Chuan Li, H. H. Li, Y. F. Zhao, Y. Y. Gong, L. Y. Niu, X. J. Liu, T. Wang, and Chang Q. Sun. *J. Mater. Chem. A*, 4: 14827–14838, 2016.
- [25] Tong Tong, Bowen He, Bicheng Zhu, Bei Cheng, and Liuyang Zhang. *Appl. Surf. Sci.*, 459:385–392, 2018.
- [26] Tanveer Hussain, H Vovusha, Thanayut Kaewmaraya, Amir Karton, V Amornkitbamrung, and Rajeev Ahuja. 29(41):415502, 2018.
- [27] Kaifei Bai, Zhen Cui, Enling Li, Yingchun Ding, Jiangshan Zheng, Yanpeng Zheng, and Chang Liu. *Mod. Phys. Lett. B*, 34(32):2050361, 2020.
- [28] Jieyuan Li, Wen Cui, Yanjuan Sun, Yinghao Chu, Wanglai Cen, and Fan Dong. *J. Mater. Chem. A*, 5:9358–9364, 2017.
- [29] Ting Xiong, Wanglai Cen, Yuxin Zhang, and Fan Dong. *ACS Catal.*, 6(4): 2462–2472, 2016.
- [30] Shuyue Wang, Chao Qian, and Shaodong Zhou. *ACS Appl. Mater. Interfaces*, 15(34):40656–40664, 2023.
- [31] Huanhuan Li, Yong Wu, Lei Li, Yinyan Gong, Lengyuan Niu, Xinjuan Liu, Tao Wang, Changqing Sun, and Can Li. *Appl. Surf. Sci.*, 457:735–744, 2018.
- [32] Dan Long, Wenlan Chen, Shaohui Zheng, Xi Rao, and Yongping Zhang. *Ind. Eng. Chem. Res.*, 59(10):4549–4556, 2020.
- [33] Wenjian Fang, Junying Liu, Lei Yu, Zhi Jiang, and Wenfeng Shangguan. *Appl. Catal. B Environ.*, 209:631–636, 2017.
- [34] Peng She, Chun Yao, Jun Li, Hegang Bao, Xiuquan Xu, and Hong Zhou. *Mater. Res. Express.*, 8(12):125006, 2021.
- [35] Yali Zhao, Yanming Lin, Guanshi Wang, Zhenyi Jiang, Ruiqin Zhang, and Chaoyuan Zhu. *Appl. Surf. Sci.*, 463:809–819, 2019.

- [36] Wei Guo, Jiajun Zhang, Guoning Li, and Chunjian Xu. *Appl. Surf. Sci.*, 470:99–106, 2019.
- [37] Mohammed Suliman, Munzir H. Suliman, Alaaldin Adam, Chanbasha Basheer, Zain H. Yamani, and Mohammad Qamar. *Mater. Lett.*, 268:127593, 2020.
- [38] Mohammed A. Suliman, Chanbasha Basheer, and Wasif Farooq. *Catalysts*, 11(10), 2021.
- [39] Hai Guo, Cheng-Gang Niu, Ya-Ya Yang, Chao Liang, Huai-Yuan Niu, Hui-Yun Liu, Lu Li, and Ning Tang. *Chem. Eng. J.*, 422:130029, 2021.
- [40] Qiu-Hui Zhu, Zhou Chen, Li-Na Tang, Yue Zhong, Xiu-Feng Zhao, Li-Zhong Zhang, and Jian-Hui Li. *Int. J. Hydrog. Energy*, 44(51):27704–27712, 2019.
- [41] Yizhang Wu, Dongxin Yang, Wei Xu, Renjie Song, Mengmeng Li, Yong Wang, Boye Zhou, Niandu Wu, Wei Zhong, Hong ling Cai, Juan Tu, Dong Zhang, and X.S. Wu. *Appl. Catal. B Environ.*, 269:118848, 2020.
- [42] Jing-He Liu, Xiang Kan, Bin Amin, Li-Yong Gan, and Yong Zhao. *Phys. Chem. Chem. Phys.*, 19:32253–32261, 2017.
- [43] Haotian Xu, Rong Xiao, Jingran Huang, Yan Jiang, Chengxiao Zhao, and Xiaofei Yang. *Chinese J. Catal.*, 42(1):107–114, 2021.
- [44] Ning Liu, Na Lu, Yan Su, Pu Wang, and Xie Quan. *Sep. Purif. Technol.*, 211:782–789, 2019.
- [45] Chongyi Ling, Li Shi, Yixin Ouyang, and Jinlan Wang. *Chem. Mater.*, 28(24):9026–9032, 2016.
- [46] Fei He, Bicheng Zhu, Bei Cheng, Jiaguo Yu, Wingkei Ho, and Wojciech Macyk. *Appl. Catal. B Environ.*, 272:119006, 2020.
- [47] E. Schrödinger. *Phys. Rev.*, 28:1049–1070, 1926.
- [48] John C. Slater. *Am. J. phys.*, 32:65–66, 1964.

-
- [49] Robert O. Jones. *Rev. Mod. Phys.*, 87:897–923, 2015.
- [50] Max Born and Robert Oppenheimer. *Ann. Phys.*, 389(20):457–484, 1927.
- [51] Douglas R. Hartree. *Math. Proc. Camb. Philos. Soc.*, 24(1):89–110, 1928.
- [52] John C. Slater. *Phys. Rev.*, 32:339, 1928.
- [53] John C. Slater. *Phys. Rev.*, 35:210, 1930.
- [54] Vladimir Fock. *Z. Phys.*, 61:126, 1930.
- [55] Walter Kohn and Lu J. Sham. *Phys. Rev.*, 140:A1133–A1138, 1965.
- [56] Pierre Hohenberg and Walter Kohn. *Phys. Rev.*, 136:B864–B871, 1964.
- [57] John W. Negeles. *Phys. Rev. C*, 1:1260–1321, 1970.
- [58] John P. Perdew, Kieron Burke, and Matthias Ernzerhof. *Phys. Rev. Lett.*, 77:3865–3868, 1996.
- [59] Peter Blaha, Karlheinz Schwarz, Fabien Tran, Robert Laskowski, Georg K. H. Madsen, and Laurence D. Marks. *Chem. Phys.*, 152(7):074101, 2020.
- [60] Jochen Heyd, Gustavo E. Scuseria, and Matthias Ernzerhof. *J. Chem. Phys.*, 118(18):8207–8215, 2003.
- [61] Jochen Heyd, Gustavo E. Scuseria, and Matthias Ernzerhof. *J. Chem. Phys.*, 124(21):219906, 2006.
- [62] Felix Bloch. *Z. Phys.*, 52:555, 1929.
- [63] H. Hellmann. *J. Chem. Phys.*, 3(1):61–61, 2004.
- [64] Donald R. Hamann, M. Schlüter, and C. Chiang. *Phys. Rev. Lett.*, 43:1494–1497, 1979.
- [65] David Vanderbilt. *Phys. Rev. B*, 41:7892–7895, 1990.
- [66] George Kresse and Daniel Joubert. *Phys. Rev. B*, 59:1758–1775, 1999.
- [67] Fabien Tran and Peter Blaha. *Phys. Rev. Lett.*, 102:226401, 2009.

- [68] Arash A. Mostofi, Jonathan R. Yates, Young-Su Lee, Ivo Souza, David Vanderbilt, and Nicola Marzari. *Comput. Phys. Commun.*, 178(9):685–699, 2008.
- [69] Nicola Marzari and David Vanderbilt. *Phys. Rev. B*, 56:12847–12865, 1997.
- [70] Stefan Grimme. *J. Comput. Chem.*, 27(15):1787–1799, 2006.
- [71] Evgenii Gross, Sergei A. Permogorov, and Boris Razbirin. *J. Phys. Chem. Solids*, 27(10):1647–1651, 1966.
- [72] Claudia Ambrosch-Draxl and Jorge O. Sofo. *Comput. Phys. Commun.*, 175(1):1–14, 2006.
- [73] Jens K. Nørskov, Jan Rossmeisl, Ashildur Logadottir, Lars Lindqvist, John R. Kitchin, Thomas Bligaard, and Hannes Jónsson. *J. Phys. Chem. B*, 108(46):17886–17892, 2004.
- [74] Jens K. Nørskov, Thomas Bligaard, Ashildur Logadottir, John R. Kitchin, Jingguang G. Chen, S. Pandelov, and Ulrich Stimming. *J. Electrochem. Soc.*, 152(3):J23, 2005.
- [75] Jan Rossmeisl, Z.-W. Qu, H. Zhu, Geert-Jan Kroes, and Jens K. Nørskov. *J. Electroanal. Chem.*, 607(1):83–89, 2007.
- [76] Paolo Giannozzi, Stefano Baroni, Nicola Bonini, Matteo Calandra, Roberto Car, Carlo Cavazzoni, Davide Ceresoli, Guido L Chiarotti, Matteo Cococcioni, and Ismaila Dabo et al. *J. Condens. Matter Phys.*, 21(39):395502, 2009.
- [77] Andre K. Geim and Konstantin S. Novoselov. *Nat. Mater.*, 6:183–191, 2007.
- [78] Daniela Pacilé, Johanna C. Meyer, Çağlar Ö. Girit, and Alex Zettl. *Appl. Phys. Lett.*, 92(13):133107, 2008.
- [79] Ali H. Reshak, Saleem A. Khan, and Sushil Auluck. *RSC Adv.*, 4:6957–6964, 2014.

-
- [80] David James Martin, Kaipei Qiu, Stephen Andrew Shevlin, Albertus Denny Handoko, Xiaowei Chen, Zhengxiao Guo, and Junwang Tang. *Angew. Chem., Int. Ed. Engl.*, 53(35):9240–9245, 2014.
- [81] Kai Dai, Dongpei Li, Luhua Lu, Qi Liu, Changhao Liang, Jiali Lv, and Guangping Zhu. *Appl. Surf. Sci.*, 314:864–871, 2014.
- [82] Jonas Wirth, Rainer Neumann, Markus Antonietti, and Peter Saalfrank. *Phys. Chem. Chem. Phys.*, 16:15917–15926, 2014.
- [83] Xiaodong Zhang, Xiao Xie, Hui Wang, Jiajia Zhang, Bicao Pan, and Yi Xie. *J. Am. Chem. Soc.*, 135(1):18–21, 2013.
- [84] S. Lu, Can Li, H.H. Li, Ya F. Zhao, Yin Y. Gong, Leng Y. Niu, Xin J. Liu, and T. Wang. *Appl. Surf. Sci.*, 392:966–974, 2017.
- [85] Jens Peter Paraknowitsch and Arne Thomas. *Energy Environ. Sci.*, 6:2839–2855, 2013.
- [86] Fazal Raziq, Yang Qu, Xuliang Zhang, Muhammad Humayun, Jing Wu, Amir Zada, Haitao Yu, Xiaojun Sun, and Liqiang Jing. *J. Phys. Chem. C*, 120(1):98–107, 2016.
- [87] Zhi Zhu, Xu Tang, Tianshuai Wang, Wenqian Fan, Zhi Liu, Chunxiang Li, Pengwei Huo, and Yongsheng Yan. *Appl. Catal. B Environ.*, 241:319–328, 2019.
- [88] Faling Ling, Wanjun Li, and Lijuan Ye. *Appl. Surf. Sci.*, 473:386–392, 2019.
- [89] Yali Zhao, Yanming Lin, Guanshi Wang, Zhenyi Jiang, Ruiqin Zhang, and Chaoyuan Zhu. *Appl. Surf. Sci.*, 463:809–819, 2019.
- [90] Dibyajyoti Ghosh, Ganga Periyasamy, and Swapan K. Pati. *J. Phys. Chem. C*, 118(28):15487–15494, 2014.
- [91] Anton Kokalj. *J. Mol. Graph. Model.*, 17(3):176–179, 1999.
- [92] Charles G. Broyden. *IMA Journal of Appl Math*, 6:222–231, 1970.

- [93] Roger Fletcher. . *Comput J*, 13(3):317–322, 1970.
- [94] Donald Goldfarb. *Math. Comp.*, 24:23–26, 1970.
- [95] David. F. Shanno. *Math. Comp.*, 24:647–656, 1970.
- [96] Suraj Gupta, Nainesh Patel, Antonio Miotello, and D.C. Kothari. *J. Power Sources*, 279:620–625, 2015.
- [97] Suraj Gupta, Maulik K. Patel, Antonio Miotello, and Nainesh Patel. *Adv. Funct. Mater.*, 30(1):1906481, 2020.
- [98] Susan Meñez Aspera, Melanie David, and Hideaki Kasai. *Jpn. J. Appl. Phys.*, 49(11R):115703, 2010.
- [99] Luis Miguel Azofra, Douglas R. MacFarlane, and Chenghua Sun. *Phys. Chem. Chem. Phys.*, 18:18507–18514, 2016.
- [100] Fang Wu, Yunfei Liu, Guanxia Yu, Dingfeng Shen, Yunlu Wang, and Erjun Kan. *J. Phys. Chem. Lett.*, 3(22):3330–3334, 2012.
- [101] Thi Thu Ha Nguyen, Minh Cam Le, and Nguyen Ngoc Ha. *Mol Simul.*, 47(1):10–17, 2021.
- [102] Sulagna Patnaik, Dipti Prava Sahoo, and Kulamani Parida. *Carbon*, 172:682–711, 2021.
- [103] Ke Wang, Jile Fu, and Ying Zheng. *Appl. Catal. B Environ.*, 254:270–282, 2019.
- [104] Jingce Bi, Lin Zhu, Junbiao Wu, Yan Xu, Zhuopeng Wang, Xia Zhang, and Yide Han. *Appl. Organomet. Chem.*, 33(10):e5163, 2019.
- [105] Jun ying Tang, Rui tang Guo, Wei guo Pan, and Wei guo Zhou. *Fuel*, 333:126280, 2023.
- [106] Jianjun Liu. *J. Phys. Chem. C*, 119(51):28417–28423, 2015.
- [107] Shen Xu, Jianying Huang, Zengxing Li, Yonggang Lei, Yingzhen Zhang, Kim Hoong Ng, and Yuekun Lai. *J. Clean. Prod.*, 402:136672, 2023.

-
- [108] Zhigang Chen, Yahui Yu, Xiaojie She, Kaixiang Xia, Zhao Mo, Hanxiang Chen, Yanhua Song, Jihua Huang, Huaming Li, and Hui Xu. *Appl. Surf. Sci.*, 495:143528, 2019.
- [109] Tsan-Chen Leung, C. L. Kao, Wan-Sheng Su, Y. J. Feng, and Che T. Chan. *Phys. Rev. B*, 68:195408, 2003.
- [110] N. Jiao, Chaoyu He, P. Zhou, C.X. Zhang, H.P. Xiao, and L.Z. Sun. *Phys. Lett. A*, 377(28):1760–1765, 2013.
- [111] Yabing Du, Xiaolong Wang, Xianqi Dai, and Wei Li. *Front. Phys.*, 10, 2022.
- [112] Thibault Sohier, Matteo Calandra, and Francesco Mauri. *Phys. Rev. B*, 96:075448, 2017.
- [113] Donald R. Hamann. *Phys. Rev. B*, 88:085117, 2013.
- [114] Hong-Zhang Wu, Li-Min Liu, and Shi-Jin Zhao. *Phys. Chem. Chem. Phys.*, 16:3299–3304, 2014.
- [115] Jian-Wen Zhao, Hong-Yue Wang, Li Feng, Jin-Ze Zhu, Jin-Xun Liu, and Wei-Xue Li. *Chem. Rev.*, 0(0):null, 2023.
- [116] Jiamao Hao, Jun Wu, Donghua Wang, Chengdeng Wang, Mengqin Luo, Lijuan Xie, Fang Zhu, Xiaoqin Yan, and Yousong Gu. *J. Phys. D: Appl. Phys.*, 56(3):035501, 2022.
- [117] Xuewen Xu, Xiaoli Ge, Xin Liu, Lanlan Li, Kun Fu, Yao Dong, Fanbin Meng, Ruihao Si, and Minghui Zhang. *Ceram. Int.*, 46(9):13377–13384, 2020.
- [118] Bao Zhu, Fusheng Zhang, Jian Qiu, Xianping Chen, Kai Zheng, Haojie Guo, Jiabing Yu, and Jiading Bao. *Mater. Sci. Semicond. Process.*, 133:105947, 2021.
- [119] Muhammad Munawar, Muhammad Idrees, Tahani A. Alrebdi, and Bin Amin. *Nanoscale Adv.*, 5:1405–1415, 2023.
- [120] Ekaterina V. Sukhanova and Zakhar I. Popov. *Phys. Chem. Chem. Phys.*, 25:32062–32070, 2023.

- [121] Xian-Hu Zha, Qing Huang, Jian He, Heming He, Junyi Zhai, Joseph S. Francisco, and Shiyu Du. *Sci. Rep.*, 6:27971, 2016.
- [122] Minghui Zhang, Ruihao Si, Xiaoyi Wu, Yao Dong, Kun Fu, Xuewen Xu, Jun Zhang, Lanlan Li, and Yue Guo. *J. Mater Sci.: Mater. Electron*, 32:19368–19379, 2021.
- [123] G. Murali, Jeevan Kumar Reddy Modigunta, Young Ho Park, Jong-Hoon Lee, Jishu Rawal, Seul-Yi Lee, Insik In, and Soo-Jin Park. *ACS Nano*, 16(9):13370–13429, 2022.
- [124] Bing He, Yang Wang, Qiaoling Zhai, Peng Qiu, Gang Dong, Xueqin Liu, Yihuang Chen, and Zhen Li. *Nanoscale*, 12:8636–8646, 2020.
- [125] Bo Wei, Wei Wang, Jianfei Sun, Qiong Mei, Zexiu An, Haijie Cao, Dandan Han, Ju Xie, Jinhua Zhan, and Maoxia He. *Appl. Surf. Sci.*, 511:145549, 2020.
- [126] Guigang Zhang, Zhi-An Lan, and Xinchun Wang. *Chem. Sci.*, 8:5261–5274, 2017.
- [127] Jose Gracia and Peter Kroll. *J. Mater. Chem.*, 19:3013–3019, 2009.
- [128] Xinchun Wang, Kazuhiko Maeda, Xiufang Chen, Kazuhiro Takanabe, Kazunari Domen, Yidong Hou, Xianzhi Fu, and Markus Antonietti. *J. Am. Chem. Soc.*, 131(5):1680–1681, 2009.
- [129] Longyan Wang, Yuanzhi Hong, Enli Liu, Zhiguo Wang, Jiahui Chen, Shuang Yang, Jingbo Wang, Xue Lin, and Junyou Shi. *Int. J. Hydrog. Energy*, 45(11):6425–6436, 2020.
- [130] Sebastian Zuluaga, Li-Hong Liu, Natis Shafiq, Sara M. Rupich, Jean-François Veyan, Yves J. Chabal, and Timo Thonhauser. *Phys. Chem. Chem. Phys.*, 17:957–962, 2015.
- [131] Xianghong Niu, Yingwei Yi, Xiaowan Bai, Jian Zhang, Zhaobo Zhou, Liang Chu, Jianping Yang, and Xing’ao Li. *Nanoscale*, 11:4101–4107, 2019.

-
- [132] Daming Zhao, Jie Chen, Chung-Li Dong, Wu Zhou, Yu-Cheng Huang, Samuel S. Mao, Liejin Guo, and Shaohua Shen. *J. Catal.*, 352:491–497, 2017.
- [133] Fang Li, Lei Cheng, Jiajie Fan, and Quanjun Xiang. *J. Mater. Chem. A*, 9: 23765–23782, 2021.
- [134] M.R.Gennero de Chialvo and A.C. Chialvo. *J. Electroanal. Chem.*, 372(1): 209–223, 1994.
- [135] Jiuqing Wen, Jun Xie, Xiaobo Chen, and Xin Li. *Appl. Surf. Sci.*, 391: 72–123, 2017.
- [136] Quanlong Xu, Liuyang Zhang, Bei Cheng, Jiajie Fan, and Jiaguo Yu. *Chem*, 6(7):1543–1559, 2020.
- [137] Rui Yang, Xiao-Huan Lv, Yin-Ti Ren, Yue-Jiao Zhang, Hu Zhang, Chen-Dong Jin, Ru-Qian Lian, Rui-Ning Wang, Peng-Lai Gong, Xing-Qiang Shi, and Jiang-Long Wang. *Phys. Rev. Materials*, 6:094011, 2022.
- [138] Qing Cao, Fabian Grote, Marleen Hubmann, and Siegfried Eigler. *Nanoscale Adv.*, 3:963–982, 2021.
- [139] Jieyuan Li, Zhiyong Zhang, Wen Cui, Hong Wang, Wanglai Cen, Grayson Johnson, Guangming Jiang, Sen Zhang, and Fan Dong. *ACS Catal.*, 8(9): 8376–8385, 2018.
- [140] Xing’an Dong, Jieyuan Li, Qian Xing, Ying Zhou, Hongwei Huang, and Fan Dong. *Appl. Catal. B Environ*, 232:69–76, 2018.
- [141] Thanh Son Bui, Palak Bansal, Byeong-Kyu Lee, Tahereh Mahvelati-Shamsabadi, and Tayyebbeh Soltani. *Appl. Surf. Sci.*, 506:144184, 2020.
- [142] Jieyuan Li, Xing’an Dong, Yanjuan Sun, Guangming Jiang, Yinghao Chu, S.C. Lee, and Fan Dong. *Appl. Catal. B Environ*, 239:187–195, 2018.
- [143] Wen Cui, Peng Chen, Lvcun Chen, Jieyuan Li, Ying Zhou, and Fan Dong. *J.Phys. Energy*, 3(3):032008, 2021.

- [144] Parsa Habibi, Tijin H.G. Saji, Thijs J.H. Vlugt, Othonas A. Moulτος, and Poulumi Dey. *Appl. Surf. Sci.*, 603:154323, 2022.
- [145] Weibin Zhang, Zhijun Zhang, Soo Ho Choi, and Woochul Yang. *Catal. Today.*, 321-322:67–73, 2019.
- [146] Zhenxing Zeng, Xie Quan, Hongtao Yu, Shuo Chen, Wonyong Choi, Bupmo Kim, and Shushen Zhang. *J. Catal.*, 377:72–80, 2019.
- [147] Bo Niu, Jiefeng Xiao, and Zhenming Xu. *J. Mater. Chem. A*, 9:472–481, 2021.
- [148] Zhitong Ge, Anchi Yu, and Rong Lu. *Mater. Lett.*, 250:9–11, 2019.
- [149] Linwei Ruan, Gengsheng Xu, Lina Gu, Cun Li, Yujun Zhu, and Yunxiang Lu. *Mater. Res. Bull.*, 66:156–162, 2015.
- [150] Ilana B. Stone, Rachel L. Starr, Norah Hoffmann, Xiao Wang, Austin M. Evans, Colin Nuckolls, Tristan H. Lambert, Michael L. Steigerwald, Timothy C. Berkelbach, Xavier Roy, and Latha Venkataraman. *Chem. Sci.*, 13: 10798–10805, 2022.
- [151] Zachary K. Goldsmith, Maxim Secor, and Sharon Hammes-Schiffer. *ACS Cent. Sci.*, 6(2):304–311, 2020.
- [152] Egill Skúlason, Gustav S. Karlberg, Jan Rossmeisl, Thomas Bligaard, Jeff Greeley, Hannes Jónsson, and Jens K. Nørskov. *Phys. Chem. Chem. Phys.*, 9:3241–3250, 2007.
- [153] Pengyu Dong, Aicaijun Zhang, Ting Cheng, Jinkang Pan, Jun Song, Lei Zhang, Rongfeng Guan, Xinguo Xi, and Jinlong Zhang. *Chinese J. Catal.*, 43(10):2592–2605, 2022.
- [154] Pengyu Dong, Chengqi Meng, Yan Yan, Beibei Zhang, Wuyou Wang, Xinguo Xi, and Jinlong Zhang. *Int. J. Hydrog. Energy*, 48(49):18670–18684, 2023.
- [155] Ivo Souza, Nicola Marzari, and David Vanderbilt. *Phys. Rev. B*, 65:035109, 2001.

-
- [156] Jun Huang. *Electrochim. Acta.*, 389:138720, 2021.
- [157] Guizhou Gu, Keyun Wang, Nanni Xiong, Zheng Li, Zhiping Fan, Shaozheng Hu, and Xiong Zou. *Dalton Trans.*, 48:5083–5089, 2019.
- [158] Yafan Yang, Arun Kumar Narayanan Nair, and Shuyu Sun. *ACS Earth Space Chem.*, 3(11):2635–2645, 2019.
- [159] Daniel D. Kemp and Mark S. Gordon. *J. Phys. Chem. A*, 112(22):4885–4894, 2008.
- [160] Yangping Zhang, Fei Gao, Dongqiong Wang, Zhuolin Li, Xiaomei Wang, Caiqin Wang, Kewang Zhang, and Yukou Du. *Coord. Chem. Rev.*, 475:214916, 2023.
- [161] Selina K. Kaiser, Zupeng Chen, Dario Faust Akl, Sharon Mitchell, and Javier Pérez-Ramírez. *Chem. Rev.*, 120(21):11703–11809, 2020.
- [162] Eric M. Lopato and Stefan Bernhard. *Energy Fuels*, 35(23):18957–18981, 2021.
- [163] Pie-Wen Chen, Kui Li, Yu-Xiang Yu, and Wie-De Zhang. *Appl. Surf. Sci.*, 392:608–615, 2017.
- [164] Kunlanan Wiranarongkorn, Kornkamol Eamsiri, Yong-Song Chen, and Amornchai Arpornwichanop. *J. CO₂ Util.*, 71:102477, 2023.
- [165] Guoping Gao, Yan Jiao, Eric R. Waclawik, and Aijun Du. *J. Am. Chem. Soc.*, 138(19):6292–6297, 2016.
- [166] Shuang Ji, Yi Li, Yongfan Zhang, and Wei Lin. *Phys. Chem. Chem. Phys.*, 25:24022–24030, 2023.
- [167] Zhe Chen, Jingxiang Zhao, Carlos R. Cabrera, and Zhongfang Chen. *Small Methods*, 3(6):1800368, 2019.
- [168] Tongwei Wu, Marko M. Melander, and Karoliina Honkala. *Curr. Opin. Electrochem.*, 42:101383, 2023.

- [169] Anmin Liu, Yanan Yang, Xuefeng Ren, Qidong Zhao, Mengfan Gao, Weixin Guan, Fanning Meng, Liguao Gao, Qiyue Yang, Xingyou Liang, and Tingli Ma. *ChemSusChem*, 13(15):3766–3788, 2020.
- [170] Zhe Chen, Jingxiang Zhao, Carlos R. Cabrera, and Zhongfang Chen. *Small Methods*, 3(6):1800368, 2019.
- [171] Xian Wang, Qiang Zhang, Weiju Hao, Chunyao Fang, Jianyang Zhou, and Jingcheng Xu. *J. Mater. Chem. A*, 10:15036–15050, 2022.
- [172] Qiang Zhang, Xian Wang, Fuchun Zhang, Chunyao Fang, Di Liu, and Qingjun Zhou. *ACS Appl. Mater. Interfaces*, 15(9):11812–11826, 2023.
- [173] Zengxi Wei, Yuezhan Feng, and Jianmin Ma. *J. Energy Chem.*, 48:322–327, 2020.
- [174] Nandha Kumar, Nicola Seriani, and Ralph Gebauer. *Phys. Chem. Chem. Phys.*, 22:10819–10827, 2020.