

## List of publications

- Papers in refereed journals and proceedings

108. R.L.H. Freire, D. Guedes-Sobrinho, A. Kiejna, J.L.F. Da Silva,  
*Comparison of Performance of van der Waals Dispersion Functionals in Description of Water and Ethanol on Transition Metal Surfaces*,  
submitted (2017).
107. T. Ossowski, J.L.F. Da Silva, A. Kiejna,  
*Water Adsorption on the Stoichiometric and Defected Fe(110) Surfaces*,  
submitted (2017).
106. D. Wiśnios, A. Kiejna, J. Korecki,  
*Towards understanding MgO/Fe interface formation: Adsorption of O and Mg atoms on an Fe(001) surface*,  
Physical Review B **96**, 115418 (2017) 1-10.
105. E. Wachowicz, T. Ossowski, A. Kiejna,  
*DFT study of stepped 4H-SiC0001 surfaces*,  
Applied Surface Science **420**, 129–135 (2017)
104. M. Lewandowski, I.M.N. Groot, Z.-H. Qin, T. Ossowski, T. Pabisiak, A. Kiejna,  
A. Pavlovska, S.Shaikhutdinov, H.-J. Freund, E. Bauer,  
*Nanoscale Patterns on Polar Oxide Surfaces*,  
Chemistry of Materials **28**, 7433 - 7443 (2016).
103. R.L.H. Freire, A. Kiejna, J.L.F. Da Silva,  
*Adsorption Properties of Water and Ethanol on Defected and Strained Transition-Metal Surfaces*,  
Physical Chemistry Chemical Physics **18**, 29526 - 29536 (2016).
102. Y. Seminovski, P. Tereshchuk, A. Kiejna, J.L.F. Da Silva,  
*The Role of the Cationic Pt Sites in the Adsorption Properties of Water and Ethanol on the Pt<sub>4</sub>/Pt(111) and Pt<sub>4</sub>/CeO<sub>2</sub>(111) Substrates: A Density Functional Theory Investigation*,  
Journal of Chemical Physics **145**, 124709 (2016) 1-10.
101. T. Pabisiak, M. J. Winiarski, T. Ossowski, A. Kiejna,  
*Adsorption of gold subnano-structures on magnetite (111) surface and their interaction with CO*,  
Physical Chemistry Chemical Physics **18**, 18169-18179 (2016).
100. K. Freindl, T. Ossowski, M. Zając, N. Spiridis, D. Wilgocka-Ślęzak, E. Madej, T. Giela,  
A. Kiejna, J. Korecki,  
*Oxygen Adsorption on the Fe(110) Surface: the Old System - New Structures*,  
Journal of Physical Chemistry C **120**, 3807-3813 (2016).
99. T. Pabisiak, M. J. Winiarski, A. Kiejna,  
*CO adsorption on small Au<sub>n</sub> (n = 1-4) structures supported on hematite: II. Adsorption on the O-rich termination of α-Fe<sub>2</sub>O<sub>3</sub>(0001) surface*,  
Journal of Chemical Physics **144**, 044705 (2016) 1-10.
98. T. Pabisiak, M. J. Winiarski, A. Kiejna,  
*CO adsorption on small Au<sub>n</sub> (n = 1-4) structures supported on hematite: I. Adsorption on iron terminated α-Fe<sub>2</sub>O<sub>3</sub>(0001) surface*,  
Journal of Chemical Physics **144**, 044704 (2016) 1-10.

97. D. Wiśnios, A. Kiejna, J. Korecki,  
*First principles study of the adsorption of MgO molecules on a clean Fe(001) surface*,  
Physical Review B **92**, 155425 (2015) 1-8.
96. R.L.H. Freire, A. Kiejna, J.L.F. Da Silva,  
*Correction to “Adsorption of Rh, Pd, Ir, and Pt on the Au(111) and Cu(111) Surfaces: A Density Functional Theory Investigation”*,  
Journal of Physical Chemistry C **119**, 21744-21744 (2015).
95. P. Tereshchuk, R.L.H. Freire, C.G. Ungureanu, Y. Seminovski, A. Kiejna, J.L.F. Da Silva,  
*The Role of Charge Transfer in the Oxidation State Change of Ce Atoms in the  $TM_{13}/CeO_2(111)$  systems ( $TM = Pd, Ag, Pt, Au$ ): A DFT+U Investigation*,  
Physical Chemistry Chemical Physics **17**, 13520-13530 (2015).
94. T. Ossowski, A. Kiejna,  
*Oxygen adsorption on Fe(110) surface revisited*,  
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93. T. Pabisiak, A. Kiejna,  
*Fe adsorption on hematite ( $\alpha-Fe_2O_3$ ) (0001) and magnetite ( $Fe_3O_4$ ) (111) surfaces*,  
Journal of Chemical Physics **141**, 134707 (2014) 1-10.
92. R.L.H. Freire, A. Kiejna, J.L.F. Da Silva,  
*Adsorption of Rh, Pd, Ir, and Pt on the Au(111) and Cu(111) Surfaces: A Density Functional Theory Investigation*,  
Journal of Physical Chemistry C **118**, 19051-19061 (2014).
91. E. Wachowicz, A. Kiejna,  
*Potential Energy Surfaces for H Adsorbed at 4H-SiC{0001} Surfaces*,  
Acta Physica Polonica A **124**, 765-767 (2013).
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84. T. Pabisiak, A. Kiejna,  
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*Effect of impurities on structural, cohesive and magnetic properties of grain boundaries in  $\alpha$ -Fe*,  
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75. T. Ossowski, A. Kiejna,  
*Density functional study of surface properties of chromium*,  
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74. T. Pabisiak, A. Kiejna,  
*Energetics of oxygen vacancies at rutile  $TiO_2(110)$  surface*,  
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*Comparative study of Ag, Au, Pd, and Pt adsorption on Mo and Ta (112) surfaces,*  
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67. A. Kiejna, G. Kresse, J. Rogal, A. De Sarkar, K. Reuter, M. Scheffler,  
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- **Review articles and chapters in books**

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- **Books**

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- **Proceedings Editor**

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• **Popularizing and history of physics papers**

11. A. Kiejna,  
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