

Списък на научните публикации на

доц. д-р Петко Стоев Петков

1. **St. Petkov, P.**, Vayssilov, G. N., Krüger, S., & Rösch, N. (2006). Structure, stability, electronic and magnetic properties of Ni₄ clusters containing impurity atoms. *Physical Chemistry Chemical Physics*, 8(11), 1282. <https://doi.org/10.1039/b518175e>
2. **Petkov, P. S.**, Vayssilov, G. N., Krüger, S., & Rösch, N. (2007). Influence of single impurity atoms on the structure, electronic, and magnetic properties of Ni₅ clusters. *Journal of Physical Chemistry A*, 111(11), 2067–2076. <https://doi.org/10.1021/jp0675431>
3. **Petkov, P. S.**, Vayssilov, G. N., Krüger, S., & Rösch, N. (2008). CO coordination at XNi₄ clusters with impurities X = H, C, O. A density functional study. *Journal of Physical Chemistry A*, 112(37), 8523–8528. <https://doi.org/10.1021/jp803348v>
4. **Petkov, P. S.**, Vayssilov, G. N., Krüger, S., & Rösch, N. (2008). Density functional study of Ni₆ clusters containing impurity atoms. *Chemical Physics*, 348(1–3), 61–68. <https://doi.org/10.1016/j.chemphys.2008.02.017>
5. Lilkova, E., Litov, L., **Petkov, P.**, Petkov, P., Markov, S., & Ilieva, N. (2010). Computer simulations of human interferon gamma mutated forms. *AIP Conference Proceedings*, 1203, 914–919. <https://doi.org/10.1063/1.3322582>
6. **Petkov, P. S.**, Petrova, G. P., Vayssilov, G. N., & Rösch, N. (2010). Saturation of small supported metal clusters by adsorbed hydrogen. a computational study on tetrahedral models of Rh₄, Ir₄, and Pt₄. *Journal of Physical Chemistry C*, 114(18), 8500–8506. <https://doi.org/10.1021/jp1014274>
7. Kolev, S. K., **Petkov, P. S.**, Rangelov, M. A., & Vayssilov, G. N. (2011). Density functional study of hydrogen bond formation between methanol and organic molecules containing Cl, F, NH₂, OH, and COOH functional groups. *Journal of Physical Chemistry A*, 115(48), 14054–14068. <https://doi.org/10.1021/jp204313f>
8. Rösch, N., Petrova, G. P., **Petkov, P. S.**, Genest, A., Krüger, S., Aleksandrov, H. A., & Vayssilov, G. N. (2011). Impurity atoms on small transition metal clusters. Insights from density functional model studies. *Topics in Catalysis*, 54(5–7), 363–377. <https://doi.org/10.1007/s11244-011-9667-0>
9. Vayssilov, G. N., Mihaylov, M., **Petkov, P. S.**, Hadjiivanov, K. I., & Neyman, K. M. (2011). Reassignment of the vibrational spectra of carbonates, formates, and related surface species on ceria: A combined density functional and infrared spectroscopy investigation. *Journal of Physical Chemistry C*, 115(47), 23435–23454. <https://doi.org/10.1021/jp208050a>
10. Aleksandrov, H., **St. Petkov, P.**, & Vayssilov, G. (2012). Computational Modeling of Coordination Chemistry of Transition Metal Cations in Zeolites and in Metal-organic Frameworks. *Current Physical Chemistry*, 2(2), 189–199. <https://doi.org/10.2174/1877946811202020189>

11. Aleksandrov, H. A., Zdravkova, V. R., Mihaylov, M. Y., **Petkov, P. S.**, Vayssilov, G. N., & Hadjiivanov, K. I. (2012). Precise identification of the infrared bands of the polycarbonyl complexes on Ni-MOR zeolite by ^{12}C ^{16}O - ^{13}C ^{18}O coadsorption and computational modeling. *Journal of Physical Chemistry C*, 116(43), 22823–22831. <https://doi.org/10.1021/jp304972u>
12. Lilkova, Elena, Nacheva, G., **Petkov, P.**, Petkov, P., Markov, S., Ilieva, N., & Litov, L. (2012). Metadynamics study of mutant human interferon-gamma forms. *Computers and Mathematics with Applications*, 64(3), 272–277. <https://doi.org/10.1016/j.camwa.2012.01.061>
13. Lukose, B., Supronowicz, B., **St. Petkov, P.**, Frenzel, J., Kuc, A. B., Seifert, G., Vayssilov, G. N., & Heine, T. (2012). Structural properties of metal-organic frameworks within the density-functional based tight-binding method. *Physica Status Solidi (B) Basic Research*, 249(2), 335–342. <https://doi.org/10.1002/pssb.201100634>
14. Lykhach, Y., Johánek, V., Aleksandrov, H. A., Kozlov, S. M., Happel, M., Skála, T., **Petkov, P. S.**, Tsud, N., Vayssilov, G. N., Prince, K. C., Neyman, K. M., Matolín, V., & Libuda, J. (2012). Water chemistry on model ceria and Pt/ceria catalysts. *Journal of Physical Chemistry C*, 116(22), 12103–12113. <https://doi.org/10.1021/jp302229x>
15. **Petkov, P. S.**, Aleksandrov, H. A., Valtchev, V., & Vayssilov, G. N. (2012). Framework stability of heteroatom-substituted forms of extra-large-pore Ge-silicate molecular sieves: The case of ITQ-44. *Chemistry of Materials*, 24(13), 2509–2518. <https://doi.org/10.1021/cm300861e>
16. **St. Petkov, P.**, Vayssilov, G. N., Liu, J., Shekhah, O., Wang, Y., Wöll, C., & Heine, T. (2012). Defects in MOFs: A thorough characterization. *ChemPhysChem*, 13(8), 2025–2029. <https://doi.org/10.1002/cphc.201200222>
17. Vayssilov, G. N., Petrova, G. P., Shor, E. A. I., Nasluzov, V. A., Shor, A. M., **Petkov, P. S.**, & Rösch, N. (2012). Reverse hydrogen spillover on and hydrogenation of supported metal clusters: Insights from computational model studies. *Physical Chemistry Chemical Physics*, 14(17), 5879–5890. <https://doi.org/10.1039/c2cp23648f>
18. Kolev, S., **Petkov, P. S.**, Rangelov, M., & Vayssilov, G. N. (2013). Ab initio molecular dynamics of Na^+ and Mg^{2+} countercations at the backbone of RNA in water solution. *ACS Chemical Biology*, 8(7), 1576–1589. <https://doi.org/10.1021/cb300463h>
19. Nacheva, G., Lilkova, E., **Petkov, P.**, Petkov, P., Ilieva, N., Ivanov, I., & Litov, L. (2014). In silico studies on the stability of human interferon-gamma mutants. *Biotechnology and Biotechnological Equipment*, 26, 200–204. <https://doi.org/10.5504/50YRTIMB.2011.0036>
20. Iglev, H., Kolev, S. K., Rossmadl, H., **Petkov, P. S.**, & Vayssilov, G. N. (2015). Hydrogen atom transfer from water or alcohols activated by presolvated electrons. *Journal of Physical Chemistry Letters*, 6(6), 986–992. <https://doi.org/10.1021/acs.jpcllett.5b00288>

21. Mallick, A., Garai, B., Addicoat, M. A., **Petkov, P. S.**, Heine, T., & Banerjee, R. (2015). Solid state organic amine detection in a photochromic porous metal organic framework. *Chemical Science*, 6(2), 1420–1425. <https://doi.org/10.1039/c4sc03224a>
22. Mihaylov, Mihail Y., Ivanova, E. Z., Aleksandrov, H. A., **Petkov, P. S.**, Vayssilov, G. N., & Hadjiivanov, K. I. (2015). Formation of N₃⁻ during interaction of NO with reduced ceria. *Chemical Communications*, 51(26), 5668–5671. <https://doi.org/10.1039/c5cc00500k>
23. Mihaylov, Mihail Y., Ivanova, E. Z., Aleksandrov, H. A., **Petkov, P. S.**, Vayssilov, G. N., & Hadjiivanov, K. I. (2015). FTIR and density functional study of NO interaction with reduced ceria: Identification of N₃⁻ and NO₂⁻ as new intermediates in NO conversion. *Applied Catalysis B: Environmental*, 176–177, 107–119. <https://doi.org/10.1016/j.apcatb.2015.03.054>
24. Wagner, M. S., Ilieva, E. D., **Petkov, P. S.**, Nikolova, R. D., Kienberger, R., & Iglev, H. (2015). Ultrafast hydrogen bond dynamics and partial electron transfer after photoexcitation of diethyl ester of 7-(diethylamino)-coumarin-3-phosphonic acid and its benzoxaphosphorin analog. *Physical Chemistry Chemical Physics*, 17(15), 9919–9926. <https://doi.org/10.1039/c4cp05727a>
25. Zeonjuk, L. L., **Petkov, P. S.**, Heine, T., Rösenthaller, G. V., Eicher, J., & Vankova, N. (2015). Are intramolecular frustrated Lewis pairs also intramolecular catalysts? A theoretical study on H₂ activation. *Physical Chemistry Chemical Physics*, 17(16), 10687–10698. <https://doi.org/10.1039/c5cp00368g>
26. Coupry, D. E., Butson, J., **Petkov, P. S.**, Saunders, M., O'Donnell, K., Kim, H., Buckley, C., Addicoat, M., Heine, T., & Szilágyi, P. (2016). Controlling embedment and surface chemistry of nanoclusters in metal-organic frameworks. *Chemical Communications*, 52(29), 5175–5178. <https://doi.org/10.1039/c6cc00659k>
27. Friedländer, S., Liu, J., Addicoat, M., **Petkov, P.**, Vankova, N., Rüger, R., Kuc, A., Guo, W., Zhou, W., Lukose, B., Wang, Z., Weidler, P. G., Pöppel, A., Ziese, M., Heine, T., & Wöll, C. (2016). Linear Chains of Magnetic Ions Stacked with Variable Distance: Ferromagnetic Ordering with a Curie Temperature above 20 K. *Angewandte Chemie - International Edition*, 55(41), 12683–12687. <https://doi.org/10.1002/anie.201606016>
28. Friedländer, S., **Petkov, P. S.**, Bolling, F., Kultaeva, A., Böhlmann, W., Ovchar, O., Belous, A. G., Heine, T., & Poppl, A. (2016). Continuous-wave single-crystal electron paramagnetic resonance of adsorption of gases to cupric ions in the Zn(II)-Doped Porous Coordination Polymer Cu_{2.965}Zn_{0.035}(btc)₂. *Journal of Physical Chemistry C*, 120(48), 27399–27411. <https://doi.org/10.1021/acs.jpcc.6b09456>
29. Fagiani, M. R., Song, X., **Petkov, P.**, Debnath, S., Gewinner, S., Schöllkopf, W., Heine, T., Fielicke, A., & Asmis, K. R. (2017). Structure and Fluxionality of B₁₃⁺ Probed by Infrared Photodissociation Spectroscopy. *Angewandte Chemie - International Edition*, 56(2), 501–504. <https://doi.org/10.1002/anie.201609766>
30. Krylov, A., Vtyurin, A., **Petkov, P.**, Senkovska, I., Maliuta, M., Bon, V., Heine, T., Kaskel, S., & Slyusareva, E. (2017). Raman spectroscopy studies of the terahertz vibrational modes

- of a DUT-8 (Ni) metal-organic framework. *Physical Chemistry Chemical Physics*, 19(47), 32099–32104. <https://doi.org/10.1039/c7cp06225g>
31. Dong, R., Han, P., Arora, H., Ballabio, M., Karakus, M., Zhang, Z., Shekhar, C., Adler, P., **Petkov, P. S.**, Erbe, A., Mannsfeld, S. C. B., Felser, C., Heine, T., Bonn, M., Feng, X., & Cánovas, E. (2018). High-mobility band-like charge transport in a semiconducting two-dimensional metal–organic framework. *Nature Materials*, 17(11), 1027–1032. <https://doi.org/10.1038/s41563-018-0189-z>
32. Hutzler, D., Brunner, C., **Petkov, P. S.**, Heine, T., Fischer, S. F., Riedle, E., Kienberger, R., & Iglev, H. (2018). Dynamics of the OH stretching mode in crystalline Ba(ClO₄)₂·3H₂O. *Journal of Chemical Physics*, 148(5). <https://doi.org/10.1063/1.5007040>
33. Kolev, S. K., **Petkov, P. S.**, Rangelov, M. A., Trifonov, D. V., Milenov, T. I., & Vayssilov, G. N. (2018). Interaction of Na⁺, K⁺, Mg²⁺ and Ca²⁺ counter cations with RNA. *Metallomics*, 10(5), 659–678. <https://doi.org/10.1039/c8mt00043c>
34. Mihaylov, Mihail Y., Ivanova, E. Z., Aleksandrov, H. A., **Petkov, P. S.**, Vayssilov, G. N., & Hadjiivanov, K. I. (2018). Species formed during NO adsorption and NO + O₂ co-adsorption on ceria: A combined FTIR and DFT study. *Molecular Catalysis*, 451, 114–124. <https://doi.org/10.1016/j.mcat.2017.11.030>
35. Popova, M., Trendafilova, I., Tsacheva, I., Mitova, V., Kyulavska, M., Koseva, N., Mihály, J., Momekova, D., Momekov, G., Aleksandrov, H. A., Marinova, S. G., **Petkov, P. S.**, Vayssilov, G. N., & Szegedi, A. (2018). Amino-modified KIT-6 mesoporous silica/polymer composites for quercetin delivery: Experimental and theoretical approaches. *Microporous and Mesoporous Materials*, 270, 40–47. <https://doi.org/10.1016/j.micromeso.2018.05.002>
36. Szegedi, Á., Shestakova, P., Trendafilova, I., Mihayi, J., Tsacheva, I., Mitova, V., Kyulavska, M., Koseva, N., Momekova, D., Konstantinov, S., Aleksandrov, H. A., St **Petkov, P.**, Koleva, I. Z., Vayssilov, G. N., & Popova, M. (2019). Modified mesoporous silica nanoparticles coated by polymer complex as novel curcumin delivery carriers. *Journal of Drug Delivery Science and Technology*, 49, 700–712. <https://doi.org/10.1016/j.jddst.2018.12.016>
37. Yoncheva, K., Merino, M., Shenol, A., Daskalov, N. T., **Petkov, P. S.**, Vayssilov, G. N., & Garrido, M. J. (2019). Optimization and in-vitro/in-vivo evaluation of doxorubicin-loaded chitosan-alginate nanoparticles using a melanoma mouse model. *International Journal of Pharmaceutics*, 556, 1–8. <https://doi.org/10.1016/j.ijpharm.2018.11.070>
38. An, Y., Kuc, A., **Petkov, P.**, Lozada-Hidalgo, M., & Heine, T. (2019). On the Chemistry and Diffusion of Hydrogen in the Interstitial Space of Layered Crystals h-BN, MoS₂, and Graphite. *Small*, 15(43), 1901722–1901722. <https://doi.org/10.1002/sml.201901722>
39. Bystrzanowska, M., **Petkov, P.**, & Tobiszewski, M. (2019). Ranking of Heterogeneous Catalysts Metals by Their Greenness. *ACS Sustainable Chemistry and Engineering*, 7(22), 18434–18443. <https://doi.org/10.1021/acssuschemeng.9b04230>

40. Ehrling, S., Senkovska, I., Bon, V., Evans, J. D., **Petkov, P.**, Krupskaya, Y., Kataev, V., Wulf, T., Krylov, A., Vtyurin, A., Krylova, S., Adichtchev, S., Slyusareva, E., Weiss, M. S., Büchner, B., Heine, T., & Kaskel, S. (2019). Crystal size: Versus paddle wheel deformability: Selective gated adsorption transitions of the switchable metal-organic frameworks DUT-8(Co) and DUT-8(Ni). *Journal of Materials Chemistry A*, 7(37), 21459–21475. <https://doi.org/10.1039/c9ta06781g>
41. Zhang, T., Qi, H., Liao, Z., Horev, Y. D., Panes-Ruiz, L. A., **Petkov, P. S.**, Zhang, Z., Shivhare, R., Zhang, P., Liu, K., Bezugly, V., Liu, S., Zheng, Z., Mannsfeld, S., Heine, T., Cuniberti, G., Haick, H., Zschech, E., Kaiser, U., Renhao D., Feng, X. (2019). Engineering crystalline quasi-two-dimensional polyaniline thin film with enhanced electrical and chemiresistive sensing performances. *Nature Communications*, 10, 4225. <https://doi.org/10.1038/s41467-019-11921-3>
42. **Petkov, P. S.**, Bon, V., Hobday, C. L., Kuc, A. B., Melix, P., Kaskel, S., Düren, T., & Heine, T. (2019). Conformational isomerism controls collective flexibility in metal-organic framework DUT-8(Ni). *Physical Chemistry Chemical Physics*, 21(2), 674–680. <https://doi.org/10.1039/c8cp06600k>
43. Yang, C., Dong, R., Wang, M., **Petkov, P. S.**, Zhang, Z., Wang, M., Han, P., Ballabio, M., Bräuninger, S. A., Liao, Z., Zhang, J., Schwotzer, F., Zschech, E., Klauss, H. H., Cánovas, E., Kaskel, S., Bonn, M., Zhou, S., Heine, T., & Feng, X. (2019). A semiconducting layered metal-organic framework magnet. *Nature Communications*, 10, 3260. <https://doi.org/10.1038/s41467-019-11267-w>
44. Popova, M., Mihaylova, R., Momekov, G., Momekova, D., Lazarova, H., Trendafilova, I., Mitova, V., Koseva, N., Mihályi, J., Shestakova, P., St. **Petkov, P.**, Aleksandrov, H. A., Vayssilov, G. N., Konstantinov, S., & Szegedi, Á. (2019). Verapamil delivery systems on the basis of mesoporous ZSM-5/KIT-6 and ZSM-5/SBA-15 polymer nanocomposites as a potential tool to overcome MDR in cancer cells. *European Journal of Pharmaceutics and Biopharmaceutics*, 142, 460–472. <https://doi.org/10.1016/j.ejpb.2019.07.021>
45. Ehrling, S., Mendt, M., Senkovska, I., Evans, J. D., Bon, V., **Petkov, P.**, Ehrling, C., Walenzus, F., Pöpl, A., & Kaskel, S. (2020). Tailoring the Adsorption-Induced Flexibility of a Pillared Layer Metal-Organic Framework DUT-8(Ni) by Cobalt Substitution. *Chemistry of Materials*, 32(13), 5670–5681. <https://doi.org/10.1021/acs.chemmater.0c01320>
46. Mihaylov, M. Y., Zdravkova, V. R., Ivanova, E. Z., Aleksandrov, H. A., **Petkov, P. S.**, Vayssilov, G. N., & Hadjiivanov, K. I. (2020). Infrared spectra of surface nitrates: Revision of the current opinions based on the case study of ceria. *Journal of Catalysis*. <https://doi.org/10.1016/j.jcat.2020.06.015>
47. Oberhofer, K. E., Musheghyan, M., Wegscheider, S., Wörle, M., Iglev, E. D., Nikolova, R. D., Kienberger, R., **Petkov, P. S.***, & Iglev, H. (2020). Individual control of singlet lifetime and triplet yield in halogen-substituted coumarin derivatives. *RSC Advances*, 10(45), 27096–27102. <https://doi.org/10.1039/d0ra05737a>

48. Popova, M., Koseva, N., Trendafilova, I., Lazarova, H., Mitova, V., Mihály, J., Momekova, D., Konstantinov, S., Koleva, I. Z., **Petkov, P. St.**, Vayssilov, G. N., Aleksandrov, H. A., & Szegedi, Á. (2021). Design of PEG-modified magnetic nanoporous silica based miltefosine delivery system: Experimental and theoretical approaches. *Microporous and Mesoporous Materials*, 310, 110664. <https://doi.org/10.1016/j.micromeso.2020.110664>
49. Abylgazina, L.; Senkovska, I.; Ehrling, S.; Bon, V.; **St. Petkov, P.**; Evans, J. D.; Krylova, S.; Krylov, A.; Kaskel, S. Tailoring Adsorption Induced Switchability of a Pillared Layer MOF by Crystal Size Engineering. *CrystEngComm* (2021) (Advanced article). <https://doi.org/10.1039/d0ce01497d>.

Глави от книга :

1. Vayssilov, G. N., Aleksandrov, H. A., Petrova, G. P., & **Petkov, P. S.** (2009). Computational Modelling of Nanoporous Materials. In *Ordered Porous Solids*. <https://doi.org/10.1016/B978-0-444-53189-6.00008-1>