

Petr Nachtigall

List of publications 1986-2008:

1. "Topological study of light sensitive photocathodes based on the Sb(NaKCs) system", J. Pancíř, I. Haslingerová, and P. Nachtigall, *Appl. Surf. Sci.* 25, 167 (1986).
2. "Topological study of the chemisorption behavior of carbon monoxide on the (112) Ni and Cu surfaces", J. Pancíř, I. Haslingerová, and P. Nachtigall, *Surf. Science* 181, 417 (1987).
3. "Topological study of the chemisorption behavior of carbon monoxide on the Pt(112) surface", J. Pancíř, I. Haslingerová, and P. Nachtigall, *Chem. Phys.* 119, 289 (1988).
4. "Quantum chemical topological study of interaction of carbon monoxide on the Pt(112) surface", J. Pancíř, I. Haslingerová, and P. Nachtigall, *Coll. Czech. Chem. Commun.* 53, 2064 (1988).
5. "Theoretical study of CO chemisorption on Ni, Cu, and Pt surfaces", J. Pancíř, I. Haslingerová, and P. Nachtigall, *Chemické Listy* 82, 1 (1988).
6. "Calculation of the Si-H bond energies for the monohydride phase of Si(100)", P. Nachtigall, K. D. Jordan, and K. C. Janda, *J. Chem. Phys.* 95, 8652 (1991).
7. "Theoretical Study of the Low-Lying Triplet and Singlet States of Diradicals: 1. Tetramethylethane", P. Nachtigall and K. D. Jordan, *J. Amer. Chem. Soc.* 114, 4743 (1992).
8. "Theoretical Study of the Low-Lying Triplet and Singlet States of Diradicals: 2. Cyclopentadienyltrimethylenemethane", P. Nachtigall, P. Dowd, and K. D. Jordan, *J. Amer. Chem. Soc.* 114, 4747 (1992).
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11. Ab initio Calculations of the Energy of Recombinative Hydrogen Desorption from the Monohydride Phase of Si(100)", P. Nachtigall, C. Sosa, K. D. Jordan, *J. Phys. Chem.* 97, 11666 (1993).
12. "Comment on "Temperature Programmed desorption of molecular hydrogen from a Si(100)-2x1 surface: Theory and experiment", P. Nachtigall and K. D. Jordan, *J. Chem. Phys.* 101, 2648 (1994).
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14. "Barriers for Hydrogen Atom Diffusion on the Si(100)-2x1 Surface", P. Nachtigall and K. D. Jordan, *J. Chem. Phys.* 102, 8249 (1995).

15. "Si adatom binding and diffusion on the Si(100) surface. Comparison of ab initio, semiempirical, and empirical potential results", A. P. Smith, J. K. Wiggs, H. Jonsson, H. Yan, L. R. Corrales, P. Nachtigall, and K. D. Jordan, *J. Chem. Phys.* 102, 1044 (1995).
16. "Investigation of the Reliability of Density Functional Methods for Studying Reactions of Gas Phase Silanes and Reactions of Hydrogen on Silicon Surfaces: H₂ Elimination Processes", P. Nachtigall, K. D. Jordan, A. P. Smith, and H. Jonsson, *J. Chem. Phys.* 104, 148 (1996).
17. "Investigation of Hybrid MCSCF-DFT Approaches for Excited States", P. Borowski, K. D. Jordan, J. Nichols, and P. Nachtigall, *Theor. Chem. Acc.* 99, 135 (1998).
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19. "Reliability of DFT methods for description of Cu sites and their interaction with NO in zeolites", D. Nachtigallová, M. Davidová, and P. Nachtigall, *Collect. Czech. Chem. Commun.* 63, 1202 (1998).
20. "Investigation of the potential energy surfaces for the ground X¹A₁ and excited C¹B₂ electronic states of SO₂", P. Nachtigall, J. Hrušák, O. Bludský, and S. Iwata, *Chem. Phys. Letters* 303, 441 (1999).
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22. "Coordination and siting of Cu⁺ ions in ZSM-5: A combined quantum mechanics/interatomic potential function study", D. Nachtigallová, P. Nachtigall, M. Sierka, and J. Sauer, *Phys. Chem. Chem. Phys.*, 1, 2019 (1999).
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