# Elenco delle Pubblicazioni

Dott. Simone Morpurgo

1. S. Morpurgo, M. Lo Jacono, P. Porta
"Pillared Hydroxycarbonates and Mixed Oxides. Part 1. Copper-Zinc-Cobalt- Aluminum System"
*J. Mater. Chem.* **4** (1994) 197-204

2. P. Porta, S. Morpurgo
"Cu-Zn-Co-Al-Cr-containing Hydrotalcite-type Anionic Clays"
*Applied Clay Sci.* **10** (1995), 31-44

3. S. Morpurgo, M. Lo Jacono, P. Porta
"Copper-Zinc-Cobalt-Chromium Hydroxycarbontes and Oxides"
*J. Solid State Chem.* **119** (1995) 246-253

4. M. Bossa, M. Colapietro, G. O. Morpurgo, S. Morpurgo, G. Portalone
"X-ray Structure and AM1 Studies of the Proton-Transfer Adduct between 2,5-Dihydroxy-p-Quinone and 4-(N,N-Dimethylamino)pyridine"
*J. Phys. Chem.* **100** (1996) 9302-9307

5. S. Morpurgo, M. Lo Jacono, P. Porta
"Copper-Zinc-Cobalt-Aluminium-Chromium Hydroxycarbontes and Oxides"
*J. Solid State Chem.* **122** (1996) 324-332

6. P. Porta, S. Morpurgo, I. Pettiti
"Characterization by X-ray absorption, X-ray powder diffraction, and magnetic susceptibility of Cu-Zn-Co-Al-containing hydroxycarbonates, oxycarbonates, oxides, and their products of reduction"
*J. Solid State Chem.* **121** (1996) 372-378

7. S. Morpurgo, M. Bossa, G. O. Morpurgo
"Ab initio Study of Intramolecular Proton Transfer Reactions in Cytosine"
*Chem. Phys. Lett.* **280** (1997) 233-238

8. G. Fierro, S. Morpurgo, M. Lo Jacono, M. Inversi, I. Pettiti
"Preparation, characterisation and catalytic activity of Cu-Zn-based manganites obtained from carbonate precursors"
*Appl. Catal. A: General* **166** (1998) 407-417

9. S. Morpurgo, M. Bossa, G. O. Morpurgo
"Critical Test of PM3-calculated Proton-Transfer Activation Energies: a Comparison with Ab initio and AM1 Calculations"
*J. Mol. Struct. (THEOCHEM)* **429** (1998) 71-80

10. S. Morpurgo, M. Bhraimi, M. Bossa, G. O. Morpurgo
"Modulation of the proton transfer equilibrium of the adducts between 2-hydroxy-p-quinones and 4-(N,N-dimethyl)aminopyridine:a semiempirical MO study"
*J. Mol. Struct. (THEOCHEM)* **429** (1998) 197-206

11. S. Morpurgo, M. Bossa, G. O. Morpurgo
"Solvent-mediated proton transfer reactions in cytosine: an ab initio study"
*Adv. Quantum Chem.* **36** (1999) 169-183

12. S. Morpurgo, M. Brahimi, M. Bossa, G. O. Morpurgo
"A theoretical study on proton transfer in the mutarotation of sugars"
*Phys. Chem. Chem. Phys.* **2** (2000) 2707-2713

13. S. Morpurgo, M. Bossa, G. O. Morpurgo
"A theoretical study of hydrogen bonding, proton transfer and kinetic isotope effects in the dimers of 2-tetrahydropyranol and in the 2-tetrahydropyranol-$H_2O$ adducts"
*Phys. Chem. Chem. Phys.* **3** (2001) 4898-4906

14. M. Bossa, S. Morpurgo, S. Stranges
"The use of ab initio and DFT calculations in the interpretation of ultraviolet photoelectron spectra: the rotational isomerism of anisole and thioanisole as a case study"
*J. Mol. Struct. (THEOCHEM)* **618** (2002) 155-164

15. S. Morpurgo, M. Bossa
"The epimerisation of 2-tetrahydropyranol catalysed by the tautomeric couples 2-pyridone/2-hydroxypyridine and formamide/formamidic acid as a model for the sugar's mutarotation: a theoretical study"
*Phys. Chem. Chem. Phys.* **5** (2003) 1181-1189

16. G. Moretti, G. Ferraris, G. Fierro, M. Lo Jacono, S. Morpurgo, M. Faticanti
"Dimeric Cu(I) species in Cu-ZSM-5 catalysts: the active sites for the NO decomposition"
*J. Catal.* **232** (2005) 476-487

17. S. Morpurgo, A. Grandi, C. Zazza, M. Bossa
"A theoretical study on the sugars' mutarotation: the epimerization of 2-tetrahydropyranol catalysed by formamidine, benzamidine and by the 2-aminopyridine/2-iminopyridine tautomeric couple"
*J. Mol. Struct. (THEOCHEM)* **729** (2005) 71-82

18. S. Morpurgo
"Group Theory and Crystal Field Theory: a simple and rigorous derivation of the spectroscopic terms generated by the $t_{2g}^2$ electronic configuration in a strong octahedral field"
*J. Chem. Education* **84** (2007) 151-155

19. A. Aurora, F. Cattruzza, C. Coluzza, C. Della Volpe, G. Di Santo, A. Flamini, C. Mangano, S. Morpurgo, P. Pallavicini, R. Zanoni
"Cathodic electrografting of versatile ligands on Si(100) as a low-impact approach for establishing a Si-C bond: A surface-coordination study of substituted 2,2'-bipyridines with $Cu^I$ ions"
*Chem. Eur. J.* **13** (2007) 1240-1250

20. S. Morpurgo, G. Moretti, M. Bossa
"A computational study on $N_2$ adsorption in Cu-ZSM-5"
*Phys. Chem. Chem. Phys.* **9** (2007) 417-424

21. M. Satta, S. Morpurgo, G. Moretti
"Long range and surface effects on the Auger parameter: electrostatic self- consistent polarization energy model"
*Surf. Interface Anal.* **40** (2008) 692-694

22. F. Calascibetta, G. Favero, G. Moretti, S. Morpurgo
"Use of the label of bottled mineral waters: a way to introduce the properties of electrolytic solutions"
*CNS La Chimica Nella Scuola*, **3** (2012) 241-246

23. S. Morpurgo, G. Moretti, M. Bossa
"Basis set effects on Cu(I) coordination in Cu-ZSM-5: a computational study"
*Theor. Chem. Acc.* **131** (2012) 1180

24. S. Morpurgo, G. Moretti, M. Bossa
"A computational study on the mechanism of NO decomposition catalyzed by Cu-ZSM-5: A comparison between single and dimeric $Cu^+$ active sites"
*J. Molec. Catal. A: Chemical* **358** (2012) 134-144

25. A. G. Marrani, M. Carboni, A. Boccia, P. Galloni, S. Morpurgo, R. Zanoni
"Reactivity of saturated hydrocarbon anchoring arms on Si(100) upon white light photoactivation: experimental evidence and theoretical insights"
*J. Phys. Chem. C* **118** (2014) 22509-22521

26. S. Morpurgo
"A DFT study on Cu(I) coordination in Cu-ZSM-5: effects of the functional choice and tuning of the ONIOM approach"
*J. Comput. Chem.* **36** (2015) 660-669

27. S. Morpurgo
"A computational study on the mechanism of NO decomposition catalyzed by short-distance Cu(I) pairs in Cu-ZSM-5"
*Molec. Catal.* **434** (2017) 96-105

28. S. Morpurgo
"The mechanism of NO and $N_2O$ decomposition catalyzed by short-distance Cu(I) pairs in Cu-ZSM-5: A DFT study on the possible role of NO and $NO_2$ in the $[CuOCu]^{2+}$ active site reduction"
*J. Catal.* **366** (2018) 189-201

29. M. De Rosa, S. Morpurgo
"A DFT study on the mechanism of NO and $N_2O$ decomposition catalysed by Cu(I) pairs in Cu-ZSM-5: Revisited reactivity at the M6 ring"
*Molec. Catal.* **522** (2022) 112206

30. M.C. Campa, D. Pietrogiacomi, C. Catracchia, S. Morpurgo, J. Olszowka, K. Mlekodaj, M. Lemishka, J. Dedecek, A. Kornas, E. Tabor
"Fe-MOR and Fe-FER as catalysts for abatement of $N_2O$ with $CH_4$ : in situ UV–vis DRS and operando FTIR study"
*Applied Catal. B: Environmental* **342** (2024) 123360

31. M. De Rosa, M.C. Campa, D. Pietrogiacomi, S. Morpurgo
"A DFT study on Cu-ZSM-5 as a catalyst for NO decomposition: possible activity of a Cu(I) pair located at the T3 tetrahedral sites"
*Molec. Catal.* **559** (2024) 114083

32. M. De Rosa, S. Morpurgo
"How to get rid of imaginary frequencies within ONIOM geometry optimizations: a DFT study on the effect of basis set and link atom distances in Cu-ZSM-5"
*Comput. Theor. Chem.* **1242** (2024) 114956