

List of Publications (* corresponding author)

2016

1. Bettinger, Holger F*; Tönshoff, Christina; Doerr, Markus and **Sanchez-Garcia, Elsa*** *“Electronically Excited States of Higher Acenes up to Nonacene: A Density Functional Theory/Multireference Configuration Interaction (DFT/MRCI) Study”*. **Journal of Chemical Theory and Computation** (2016), 12, 305–312.
2. Costa, Paolo; Lohmiller, Thomas; Trosien, Iris; Savitsky, Anton*; Lubitz, Wolfgang; Fernández-Oliva, Miguel; **Sanchez-Garcia, Elsa*** and Sander, Wolfram*. *“Light and Temperature Control Of the Spin State of Bis(p-methoxy-phenyl)carbene: a Magnetically Bistable Carbene”* **Journal of the American Chemical Society** (2016), 138, 1622–1629.
3. Henkel, Stefan; Costa, Paolo; Klute, Linda; Sokkar, Pandian; Fernandez-Oliva, Miguel; Thiel, Walter; **Sanchez-Garcia, Elsa*** and Sander, Wolfram* *“Switching the Spin State of Diphenylcarbene via Halogen Bonding”* **Journal of the American Chemical Society** (2016), 138, 1689–1697.
4. Knorr, Johannes; Sokkar, Pandian; Schott, Sebastian; Costa, Paolo; Thiel, Walter; Sander, Wolfram; **Sanchez-Garcia, Elsa*** and Nuernberger, Patrick* *“Competitive Solvent-Molecule Interactions Govern the Primary Processes of Diphenylcarbene in Solvent Mixtures”* **Nature Communications** (2016), 7:12968.
5. Arumughan , Anup; Roske , Yvette; Barth , Carolin; Forero, Laura; Bravo-Rodriguez, Kenny; Redel , Alexandra; Faelber, Katja; Rau , Kirstin; Mielke , Thorsten; Daumke , Oliver; **Sanchez-Garcia, Elsa**; Rocks, Oliver; Panakova , Daniela; Heinemann, Udo and Wanker, Erich *“Quantitative interaction mapping reveals an extended ubiquitin regulatory domain in ASPL that disrupts functional p97 hexamers”* **Nature Communications** (2016), 7:13047.
6. Trusch, Franziska; Kowski, Klaus; Bravo-Rodriguez, Kenny; Beuck, Christine; Sowislok, Andrea; Wettig, Burkhard; Matena, Anja; **Sanchez-Garcia, Elsa**; Meyer, Hemmo; Schrader, Thomas; and Bayer, Peter *“Molecular tweezers target a protein-protein interface and thereby modulate complex formation”* (2016), **Chemical Communications**, DOI: 10.1039/c6cc08039a.
7. Sprengel, Andreas; Lill, Pascal; Stegemann, Pierre; Bravo-Rodriguez, Kenny; Schöneweiß, Elisa-Charlott; Merdanovic, Melisa; Gudnason, Daniel; Aznauryan, Mikayel; Gamrad, Lisa; Barcikowski, Stephan; **Sanchez-Garcia, Elsa**; Birkedal, Victoria; Gatsogiannis, Christos; Ehrmann, Michael and Sacca, Barbara. *“Tailored protein encapsulation into a DNA host using geometrically organized supramolecular interactions”* Accepted at **Nature Communications**.

2015

8. Costa, Paolo; Trosien, Iris; Fernandez-Oliva, Miguel; Sanchez-Garcia, Elsa*; Sander, Wolfram*. "The Fluorenyl Cation" **Angewandte Chemie** (2015), 54, 2656-2660. VIP publication and **Journal Cover**.
9. Sokkar, Pandian; Boulanger, Eliot; Thiel, Walter; Sanchez-Garcia, Elsa*. "Hybrid Quantum Mechanics/Molecular Mechanics/Coarse-Grained Modeling: A Triple-Resolution Approach for Biomolecular Systems" **Journal of Chemical Theory and Computation** (2015), 11, 1809–1818. **Journal Cover**.
10. Hanke, Kenny; Kaufmann, Martin; Schwaab, Gerhard; Havenith, Martina; Wolke, Conrad T.; Gorlova, Olga; Johnson, Mark A.; Kar, Bishnu; Sander, Wolfram; Sanchez-Garcia, Elsa "Understanding the Ionic Liquid [NC4111][NTf2] from Individual Building Blocks: An IR-spectroscopic Study" **Physical Chemistry Chemical Physics** (2015), 17, 8518-8529.
11. Bravo-Rodriguez, Kenny; Klopries, Stephan; Koopmans, Kyra R. M.; Sundermann, Uschi; Yahiaoui, Samir; Arens, Julia; Kushnir, Susanna; Schulz, Frank*; Sanchez-Garcia, Elsa*. "Substrate Flexibility of a Mutated Acyltransferase Domain: Implications for Polyketide Biosynthesis". **Chemistry & Biology**. (2015), 22, 1425–1430. **Journal Cover**.
12. Klopries, Stephan; Bravo-Rodriguez, Kenny; Koopmans, Kyra R. M.; Sundermann, Uschi; Yahiaoui, Samir; Arens, Julia; Kushnir, Susanna; Sanchez-Garcia, Elsa* and Schulz, Frank*. "Data in support of Substrate Flexibility of a Mutated Acyltransferase Domain: Implications for Polyketide Biosynthesis". **Data in Brief** (2015), 5, 528–536.
13. Lopes, Dahabada H. J.; Attar, Aida; Nair, Gayatri; Hayden, Eric; Du, Zhenming; McDaniel, Kirsten; Dutt, Som; Bandmann, Heinz; Bravo-Rodriguez, Kenny; Mittal, Sumit; Klärner, Frank; Wang, Chunyu; Sanchez-Garcia, Elsa; Schrader, Thomas; Bitan, Gal. "Molecular Tweezers Inhibit Islet Amyloid Polypeptide Assembly and Toxicity by a New Mechanism" **ACS Chemical Biology**. (2015), 10, 1555–1569. **Journal Cover**.
14. Lump, Edina; Castellano, Laura M.; Meier, Christoph; Seeliger, Janine; Erwin, Nelli; Sperlich, Benjamin; Stürzel, Christina M.; Usmani, Shariq; Hammond, Rebecca M.; von Einem, Jens; Gerold, Gisa; Kreppel, Florian; Bravo-Rodriguez, Kenny; Pietschmann, Thomas; Holmes, Veronica M.; Weissman, Drew; Sowislok, Andrea; Wettig, Burkhard; Heid, Christian; Kirchhoff, Frank; Weil, Tanja; Klaerner, Frank-Gerrit; Schrader, Thomas; Bitan, Gal; Sanchez-Garcia, Elsa; Winter, Roland; Shorter, James; Münch, Jan. "A Molecular Tweezer Antagonizes Seminal Amyloids and HIV Infection". **eLife**, (2015), 4:e05397.
15. Martinez Gonzalez, Marco; Bravo-Rodriguez, Kenny; Suardíaz, Reynier; García de la Vega, José M.; Montero, Luis A. and Sanchez-Garcia, Elsa and Crespo-Otero, Rachel "Complexes of Nitric Oxide with Water and Imidazole". **Theoretical Chemistry Accounts** (2015) 134:88.

2014

16. Costa, Paolo; Fernandez-Oliva, Miguel; Sanchez-Garcia, Elsa* and Sander, Wolfram * “*The Highly Reactive Benzhydryl Cation Isolated and Stabilized in Water Ice*” **Journal of the American Chemical Society** (2014), 136, 15625–15630. Featured in *JACS Spotlights* and **Journal Cover**.
17. Sander, Wolfram*; Roy, Saonli; Bravo-Rodriguez, Kenny; Grote, Dirk and Sanchez-Garcia, Elsa* “*The Benzylperoxy Radical as a Source of Hydroxyl and Phenyl Radicals*”, **Chemistry–A European Journal** (2014), 20, 12917–12923.
18. Bravo-Rodriguez, Kenny; Ismail-Ali, Ahmed F.; Klopries, Stephan; Kushnir, Susanna; Ismail, Shehab; Fansa, Eyad K.; Wittinghofer, Alfred; Schulz, Frank* and Sanchez-Garcia, Elsa* “*Predicted Incorporation of Non-Native Substrates by a Polyketide Synthase Yields Bioactive Natural Product Derivatives*”, **ChemBioChem** (2014), 15, 1991–1997.
19. Crespo-Otero, Rachel; Mardyukov, Artur; Sanchez-Garcia, Elsa; Sander, Wolfram and Barbatti, Mario “*Photo-stability of Peptide-bond Aggregates: N-methylformamide Dimers*”, **Physical Chemistry Chemical Physics** (2014), 16 (35), 18877–18887.
20. Klopries, Stephan; Koopmans, Kyra R. M.; Sanchez-Garcia, Elsa* and Schulz, Frank*. “*Biosynthesis with Fluorine*”. **ChemBioChem** (2014), 15, 495–497.
21. Merten, Christian; Li, Fee; Bravo-Rodriguez, Kenny; Sanchez-Garcia, Elsa; Xu, Yunjie and Sander, Wolfram. “*Solvent-induced Conformational Changes in Cyclic Peptides: A Vibrational Circular Dichroism Study*”. **Physical Chemistry Chemical Physics** (2014), 16(12), 5627–5633.

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22. Li, Fee; Bravo-Rodriguez, Kenny; Fernandez-Oliva, Miguel; Ramirez-Anguita, Juan M.; Merz, Klaus; Winter, Manuela; Lehmann, Christian W.; Sander, Wolfram* and Sanchez-Garcia, Elsa*. “*Stereochemistry Rules: a Single Stereocenter Changes the Conformation of a Cyclic Tetrapeptide*”. **Journal of Physical Chemistry B** (2013), 117, 10785–10791.
23. Hernández-Rodríguez, Erix W.; Montero Alejo, Ana L.; López, Rafael; Sanchez-Garcia, Elsa; Montero, Luis A. and García de la Vega, José M. “*Electron Density Deformations provide new Insights into the Spectral Shift of Rhodopsins*”. **Journal of Computational Chemistry** (2013) 34, 2460–2471 (inside cover).
24. Dutt, Som; Wilch, Constanze; Gersthagen, Thomas; Talbiersky, Peter; Bravo-Rodriguez, Kenny; Hanni, Matti; Sanchez-Garcia, Elsa*; Ochsenfeld, Christian*; Klärner, Frank* and Schrader, Thomas*. “*Molecular Tweezers with Varying Anions: A Comparative Study*”. **Journal of Organic Chemistry** (2013), 78, 6721–6734.

25. Li, Fee; Bravo-Rodriguez, Kenny; Phillips, Charlotte; Seidel, Ruediger; Wieberneit, Florian; Stoll, Raphael; Doltsinis, Nikos L.; Sanchez-Garcia, Elsa* and Sander, Wolfram*. "Conformation and Dynamics of a Cyclic Disulfide-Bridged Peptide: Effects of Temperature and Solvent". **Journal of Physical Chemistry B** (2013), 117, 3560–3570.
26. Bier, David; Rose, Rolf; Bravo-Rodriguez, Kenny; Bartel, Maria; Ramirez-Anguita, Juan Manuel; Dutt, Som; Wilch, Constanze; Klärner, Frank; Sanchez-Garcia, Elsa*; Schrader, Thomas* and Ottmann, Christian*. "Molecular Tweezers Modulate 14-3-3 Protein-protein Interactions". **Nature Chemistry** (2013), 5, 234–239.
27. Sundermann, Uschi; Bravo-Rodriguez, Kenny; Klopries, Stephan; Kushnir, Susanna; Gomez, Hansel; Sanchez-Garcia, Elsa* and Schulz, Frank*. "Enzyme-Directed Mutasynthesis: A Combined Experimental and Theoretical Approach to Substrate Recognition of a Polyketide Synthase". **ACS Chemical Biology** (2013), 8, 443–450.
28. Crespo-Otero, Rachel; Bravo-Rodriguez, Kenny; Roy, Saonli; Benighaus Tobias; Thiel, Walter; Sander, Wolfram and Sanchez-Garcia, Elsa*. "Interactions of Aromatic Radicals with Water". **ChemPhysChem**, special issue (2013), 14, 805–811.
29. Crespo-Otero, Rachel; Mardyukov, Artur; Sanchez-Garcia, Elsa; Barbatti, Mario and Sander, Wolfram. "Photochemistry of N-Methylformamide: Matrix Isolation and Nonadiabatic Dynamics". **ChemPhysChem**, special issue (2013), 14, 827–836.

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32. Hernández-Rodríguez, Erix W.; Sanchez-Garcia, Elsa*; Crespo-Otero, Rachel; Montero Alejo, Ana L.; Montero, Luis A. and Thiel, Walter. "Understanding Rhodopsin Mutations Linked to the Retinitis Pigmentosa Disease: A QM/MM and DFT/MRCI Study". **Journal of Physical Chemistry B** (2012), 116, 1060–1076.

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33. Metzelthin, Anja; Sánchez-García, Elsa; Birer, Özgür; Schwaab, Gerhard; Thiel, Walter; Sander, Wolfram and Havenith, Martina. "Acetylene•••Furan Trimer Formation at 0.37 K as a Model for Ultracold Aggregation of Non- and Weakly Polar Molecules". **ChemPhysChem** (2011), 12(10), 2009–2017.
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39. Bettinger, Holger F.; Kar, Tapas and Sánchez-García, Elsa. "The Borazine and Benzene Homo- and Heterodimers". **Journal of Physical Chemistry A** (2009), 113, 3353–3359.
40. Mardyukov, Artur; Sánchez-García, Elsa and Sander, Wolfram. "Matrix Isolation and Ab Initio Study of the Noncovalent Complexes between Formamide and Acetylene". **Journal of Physical Chemistry A** (2009), 113, 1086–1095.
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49. Sánchez-García, Elsa; George, Lisa; Montero, Luis A. and Sander, Wolfram. "1:2 Formic Acid/Acetylene Complexes: *Ab initio* and Matrix Isolation Studies of Weakly Interacting Systems". **Journal of Physical Chemistry A** (2004), 108(52), 11846–11854.
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