

LIGAND UNBINDING VIA MULTIPLE REACTION PATHWAYS



NICOLAUS COPERNICUS UNIVERSITY

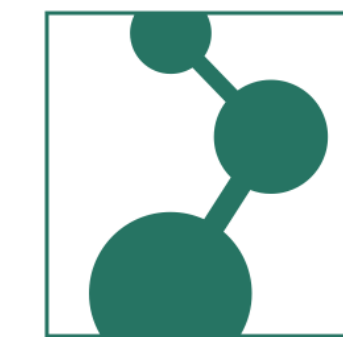
Institute of Physics | Simulational Physics

Jakub Rydzewski¹ and Omar Valsson²

¹*Institute of Physics, Nicolaus Copernicus University, Grudziadzka 5, 87-100 Torun, Poland*

²*Max Planck Institute for Polymer Research, Mainz, Germany*

MAX PLANCK INSTITUTE
FOR POLYMER RESEARCH



INTRODUCTION

METHODOLOGY

CONCLUSIONS

References

- [1] J. Rydzewski & W. Nowak. *Phys. Life Rev.* doi.org/10.1016/j.plrev.2017.03.003 (2017).
[2] W. Nowak. *Handbook of Computational Chemistry* 2nd ed. J. Leszczynski, Springer (2017).
[3] J. Rydzewski & W. Nowak. *J. Chem. Phys.* 143, 09B617_1 (2015).
[4] J. Rydzewski & W. Nowak. *J. Chem. Theory Comp.* 12, 2110 (2016).

[5] J. Rydzewski & W. Nowak. *Sci. Rep.*, submitted (2017).

[6] J. Rydzewski, R. Jakubowski, W. Nowak & H. Grubmueller, in preparation (2017).

Contact

- JR – jr@fizyka.umk.pl
● WN – wiesiek@fizyka.umk.pl

Acknowledgments

JR acknowledges funding (grants no. 2015/19/N/ST3/02171 and 2016/20/T/ST3/00488)) from National Science Centre, Poland and UMK grants 2406-F, 2539-F. The results were obtained using Interdisciplinary Centre for Modern Technologies computational facilities, NCU Torun, Poland.