Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

**Combining first principles and replica exchange for the structure of two large peptides: Ac-Ala$_{19}$-LysH$^+$ vs. Ac-LysH$^+$-Ala$_{19}$**[1] FRANZISKA SCHUBERT, MARIANA ROSSI, CARSTEN BALDAUF, VOLKER BLUM, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, D-14195 Berlin — Predicting the structure of peptides requires a high accuracy for "weak" interactions. We here focus on the predominant structure types of two alanine-based peptides *in vacuo* from first principles and in comparison to experimental IR spectroscopy[1]: Ac-Ala$_{19}$-LysH$^+$, which is expected to be $\alpha$-helical [1,2], and Ac-LysH$^+$-Ala$_{19}$, where globular monomers, helical dimers, and helices with non-standard protonation sites are expected [2]. Despite supposedly very different conformers, Ac-LysH$^+$-Ala$_{19}$ and Ac-Ala$_{19}$-LysH$^+$ yield very similar experimental IR spectra in the ≈1000-2000 cm$^{-1}$ wavenumber range. We utilize a two-stage structure search approach: we begin by a force-field based replica exchange molecular dynamics (REMD) scan followed by further REMD scans based on density functional theory with the van der Waals corrected [3] PBE functional. We suggest plausible candidates for all likely structure prototypes. Helix-turn-helix motifs emerge as the most likely candidates and explain a subtle peak shift in experiment. [1] M. Rossi *et al.*, JPCL **1**, 3465 (2010); [2] M. Jarrold, PCCP **9**, 1659 (2007); [3] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).

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Date submitted: 11 Nov 2011 Electronic form version 1.4