Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

(Un)folding of a high-temperature stable polyalanine helix from first principles VOLKER BLUM, MARIANA ROSSI, ALEX TKATCHENKO, MATTHIAS SCHEFFLER, Fritz Haber Institute, D-14195 Berlin, Germany — Peptides *in vacuo* offer a unique, well-defined testbed to match experiments directly against first-principles approaches that predict the intramolecular interactions that govern peptide and protein folding. In this respect, the polyalanine-based peptide Ac-Ala_{15}-$LysH^+$ is particularly interesting, as it is experimentally known to form helices *in vacuo*, with stable secondary structure up to ≈ 750 K [1]. Room-temperature folding and unfolding timescales are usually not accessible by direct first-principles simulations, but this high T scale allows a rare direct first-principles view. We here use van der Waals corrected [2] density functional theory in the PBE generalized gradient approximation as implemented in the all-electron code FHI-aims [3] to show by Born-Oppenheimer *ab initio* molecular dynamics that Ac-Ala_{15}-$LysH^+$ indeed unfolds rapidly (within a few ps) at T=800 K and 1000 K, but not at 500 K. We show that the structural stability of the α helix at 500 K is critically linked to a correct van der Waals treatment, and that the designed $LysH^+$ ionic termination is essential for the observed helical secondary structure. [1] M. Kohtani *et al.*, JACS **126**, 7420 (2004). [2] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009). [3] V. Blum *et al*, Comp. Phys. Comm. **180**, 2175 (2009).

Volker Blum
Fritz Haber Institute, D-14195 Berlin, Germany

Date submitted: 20 Nov 2009 Electronic form version 1.4