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Role of van der Waals interactions for the intrinsic stability of polyalanine helices ALEXANDRE TKATCHENKO, VOLKER BLUM, Fritz-Haber-Institut der MPG, Berlin, Germany, JOEL IRETA, Dep. Quimica, UAM-Iztapalapa, Mexico, MATTHIAS SCHEFFLER, Fritz-Haber-Institut der MPG, Berlin, Germany — The helical motif is an ubiquitous conformation adopted by aminoacid residues in a protein structure and helix formation is the simplest example of the protein folding process. How stable is the folded peptide helix in comparison to a random coil structure? What are the interactions responsible for stabilizing the helical conformation? Answering these questions has thus a direct implication for understanding protein folding. In this work we use density functional theory (DFT) augmented with a non-empirical correction for van der Waals (vdW) forces to study the stability of alanine polypeptide helices *in vacuo*. We find a large stabilization of the native helical forms when vdW correction is used. It amounts to 121%, 157% and 83% on top of the Perdew-Burke-Ernzerhof (PBE) functional in the case of infinite α, π and 3_{10} helices, respectively. Thus, the experimentally observed α helix is significantly stabilized by vdW forces both over the fully extended and the 3_{10} conformations. Our findings also suggest an explanation to the remarkable stability of gas-phase alanine helices up to high temperatures [M. Kohtani *et al.* JACS 126, 7420 (2004)].

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