**Calculation of forces in the KKR method** JONAS FRIEDRICH
SCHAEFER, MICHAEL CZERNER, CHRISTIAN HEILIGER, Justus-Liebig Universitt Giessen — Although the general method of calculating forces on atomic nuclei
in the KKR formalism seems to be simple, a closer investigation reveals major challenges:
First, Hellmann-Feynman forces are very sensitive to small deviations from a spherical core electron density. Given that spherical symmetry is a requirement for fast
convergence of the angular momentum expansion, this contribution needs special
treatment. Further, the expression for the interstitial space contribution (i.e., the
space outside the Muffin-Tin spheres) is highly sensitive to the angular momentum
cut-off, too.
We present quantitative studies to the aforementioned problems and trace them back
to the underlying mathematical expressions. Based thereupon, we discuss possible
improvements to the calculational scheme.

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