

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Lattice dynamics of the light actinides** JOHANN BOUCHET, CEA —

Despite general interest in  $f$ -electron elements, details about their phonon-dispersion relationships are very limited. But recently, a new hope has emerged with several works, using inelastic x-ray scattering, mostly on U and Pu. Nevertheless all this experimental issues show that theoretical works are needed to tackle the  $f$  electrons systems elastic properties. Unfortunately these calculations are far from being straightforward. Theoretically, the most important problem comes from the difficulty to treat correctly the  $f$ -electrons and the relativistic effects needed in such heavy materials. The lattice dynamics of  $\alpha$ -uranium are known for almost 30 years, but until now any theory has been able to successfully reproduce these experimental data. Here we present the first *ab-initio* phonon spectrum of  $\alpha$ -U[1]. We compare our spectrum obtained at 0 K with the neutron-scattering data obtained at room temperature with a particular attention to its anomalies. Then we predict the behavior of lattice dynamics of uranium as a function of pressure. We have also calculated the phonon spectra and the thermodynamic properties of Th, as the linear thermal expansion or specific heats[2], and the elastic properties of Th, Pa and U. [1]J. Bouchet submitted to Phys. Rev. Letter. [2]J. Bouchet, F. Jollet and G. Zerah, Phys. Rev. B 74 064637

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Date submitted: 05 Dec 2006

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