Niobium (tests by Matteo Salvetti / Nicola Marzari @ MIT Jun 2007)

We have tested three different pseudo-potentials for niobium, with the results reported in table I. Elastic constants were obtained by imposing deformations to a two atoms unit cell (ibrav=0). Niobium is characterized by a bcc structure and by a cubic stiffness matrix fully described by three independent elastic constants

$$\mathbf{C} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

In all our tests, we used a k-point grid 12x12x12, cold smearing of 0.03 Ry, and checked for convergence the elastic constants with more accurate grids (16x16x16 and 20x20x20).

We used a kinetic energy cutoff for wavefunctions of 40 Ry and a kinetic energy cutoff for charge density and potential of 400 Ry (all these are extremely conservative choices)

All the pseudopotentials predict a C_{44} elastic constant that is too soft (this is work in progress), with PBE giving slightly better C_{44} values compared to LDA and PW91.

Table I

Niobium				
Parameter	Experimental value	Calculated value PBE [Nb.pbe-nsp-van.UPF]	Calculated value PW91 [Nb.pw91-nsp-van.UPF]	Calculated value LDA [Nb.lda.UPF] de Gironcoli
Lattice parameter *a*	6.24 au	6.2513 au	6.2490 au	6.135 au
C_{11} [Mbar]	2.2570	2.41029	-	2.76186
C_{12} [Mbar]	1.3320	1.37483	-	1.48258
B_m [Mbar]	1.730	1.71998	1.72256	1.90894
C_{44} [Mbar]	0.3020	0.11029	0.0725	0.04750

B_m = bulk modulus