Hubbard U

Hubbard U is a parameter which allows correlation effects to be included in density functional calculations using the LDA+U approach. Materials Studio considers the *Hubbard U* value as a floating point quanity defined per valence orbital (of *s*, *p*, *d*, or *f* type) that is passed to the computa onal server such as CASTEP and used for electronic structure calcula ons.

Typically, the default values of Hubbard U are set when a structure is being prepared as input for a calculation, using for example CASTEP, according to the table below.

Note: Elements and angular momenta not mentioned here are assigned zero Hubbard U values by default.

Element Name	Atomic number	Angular Momentum	Hubbard U
Sc	21	d	2.5 eV
Ti	22	d	2.5 eV
V	23	d	2.5 eV
Cr	24	d	2.5 eV
Mn	25	d	2.5 eV
Fe	26	d	2.5 eV
Co	27	d	2.5 eV
Ni	28	d	2.5 eV
Cu	29	d	2.5 eV
Y	39	d	2.0 eV
Zr	40	d	2.0 eV
Nb	41	d	2.0 eV
Mo	42	d	2.0 eV
Tc	43	d	2.0 eV
Ru	44	d	2.0 eV
Rh	45	d	2.0 eV
Pd	46	d	2.0 eV
Ag	47	d	2.0 eV
Cd	48	d	2.0 eV
La	57	f	6.0 eV
Ce	58	f	6.0 eV
Pr	59	f	6.0 eV
Nd	60	f	6.0 eV
Pm	61	f	6.0 eV
Sm	62	f	6.0 eV
Eu	63	f	6.0 eV
Gd	64	f	6.0 eV
Tb	65	f	6.0 eV
Dy	66	f	6.0 eV
Ho	67	f	6.0 eV
Er	68	f	6.0 eV

Element Name	Atomic number	Angular Momentum	Hubbard U
Tm	69	f	6.0 eV
Yb	70	f	6.0 eV
Fr	87	f	2.0 eV
Ra	88	f	2.0 eV
Ac	89	f	2.0 eV
Th	90	f	2.0 eV
Pa	91	f	2.0 eV
U	92	f	2.0 eV
Np	93	f	2.0 eV
Pu	94	f	2.0 eV
Am	95	f	2.0 eV
Cm	96	f	2.0 eV
Bk	97	f	2.0 eV
Cf	98	f	2.0 eV
Es	99	f	2.0 eV
Fm	100	f	2.0 eV
Md	101	f	2.0 eV
No	102	f	2.0 eV