

Periodic table of Tersoff-Brenner-like bond order potentials

1																	18	
1	1 H Hydrogen															2 He Helium		
2	3 Li Lithium	4 Be Beryllium											5 B Boron	6 C Carbon	7 N Nitrogen	8 O Oxygen	9 F Flourine	10 Ne Neon
3	11 Na Sodium	12 Mg Magnesium											13 Al Aluminium	14 Si Silicon	15 P Phosphorus	16 S Sulphur	17 Cl Chlorine	18 Ar Argon
4	19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titanium	23 V Vanadium	24 Cr Chromium	25 Mn Manganese	26 Fe Iron	27 Co Cobalt	28 Ni Nickel	29 Cu Copper	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Selenium	35 Br Bromine	36 Kr Krypton
5	37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdenum	43 Tc Technetium	44 Ru Ruthenium	45 Rh Rhodium	46 Pd Palladium	47 Ag Silver	48 Cd Cadmium	49 In Indium	50 Sn Tin	51 Sb Antimony	52 Te Tellurium	53 I Iodine	54 Xe Xenon
6	55 Cs Caesium	56 Ba Barium	57-71 La-Lu Lanthanide	72 Hf Hafnium	73 Ta Tantalum	74 W Tungsten	75 Re Rhenium	76 Os Osmium	77 Ir Iridium	78 Pt Platinum	79 Au Gold	80 Hg Mercury	81 Tl Thallium	82 Pb Lead	83 Bi Bismuth	84 Po Polonium	85 At Astatine	86 Rn Radon
7	87 Fr Francium	88 Ra Radium	89-103 Ac-Lr Actinide	104 Rf Rutherfordium	105 Db Dubnium	106 Sg Seaborgium	107 Bh Bohrium	108 Hs Hassium	109 Mt Meitnerium	110 Ds Darmstadtium	111 Rg Roentgenium	112 Uub Ununbium	113 Uut Ununtrium	114 Uuq Ununquadium	115 Uup Ununpentium	116 Uuh Ununhexium	117 Uus Ununseptium	118 Uuo Ununoctium
	57 La Lanthanum	58 Ce Cerium	59 Pr Praseodymium	60 Nd Neodymium	61 Pm Promethium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dysprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutetium			
	89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Americium	96 Cm Curium	97 Bk Berkelium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendelevium	102 No Nobelium	103 Lr Lawrencium			

Index of potentials

Note: This is not a complete list of all existing Tersoff-like potentials. Update requests can be sent to jesper.byggmastar@helsinki.fi

H–X

- H–H [Brenner(1990)]
- H–H [Brenner et al.(2002)Brenner, Shenderova, Harrison, Stuart, Ni, and Sinnott]
- H–C [Brenner(1990)]
- H–C [Brenner et al.(2002)Brenner, Shenderova, Harrison, Stuart, Ni, and Sinnott]
- H–O [Ni et al.(2004)Ni, Lee, and Sinnott]
- H–Be [Björkas et al.(2009)Björkas, Juslin, Timko, Vörtler, Nordlund, Henriksson, and Erhart]
- H–Fe [Kuopanportti et al.(2016)Kuopanportti, Hayward, Fu, Kuronen, and Nordlund]
- H–W [Juslin et al.(2005)Juslin, Erhart, Träskelin, Nord, Henriksson, Nordlund, Salonen, and Albe]

Be–X

- Be–Be [Björkas et al.(2009)Björkas, Juslin, Timko, Vörtler, Nordlund, Henriksson, and Erhart]
- Be–C [Björkas et al.(2009)Björkas, Juslin, Timko, Vörtler, Nordlund, Henriksson, and Erhart]
- Be–H [Björkas et al.(2009)Björkas, Juslin, Timko, Vörtler, Nordlund, Henriksson, and Erhart]
- Be–O Byggmästar et al. Article in preparation, parameters available on request.
- Be–W [Björkas et al.(2010)Björkas, Henriksson, Probst, and Nordlund]

C–X

- C–C [Tersoff(1988b)]
- C–C [Brenner(1990)]
- C–C [Brenner et al.(2002)Brenner, Shenderova, Harrison, Stuart, Ni, and Sinnott]
- C–C [Erhart and Albe(2005)]
- C–H [Brenner(1990)]
- C–H [Brenner et al.(2002)Brenner, Shenderova, Harrison, Stuart, Ni, and Sinnott]
- C–O [Ni et al.(2004)Ni, Lee, and Sinnott]
- C–Si [Erhart and Albe(2005)]
- C–Fe [Henriksson et al.(2013)Henriksson, Björkas, and Nordlund]
- C–Fe [Henriksson and Nordlund(2009)]
- C–Cr [Henriksson et al.(2013)Henriksson, Björkas, and Nordlund]
- C–W [Juslin et al.(2005)Juslin, Erhart, Träskelin, Nord, Henriksson, Nordlund, Salonen, and Albe]
- C–Pt [Albe et al.(2002a)Albe, Nordlund, and Averback]

N–X

- N–N [Nord et al.(2003)Nord, Albe, Erhart, and Nordlund]
- N–Ga [Nord et al.(2003)Nord, Albe, Erhart, and Nordlund]
- N–W [Polvi et al.(2016)Polvi, Heinola, and Nordlund]

O–X

- O–O [Ni et al.(2004)Ni, Lee, and Sinnott]
- O–O [Erhart et al.(2006)Erhart, Juslin, Goy, Nordlund, Müller, and Albe]
- O–O [Munetoh et al.(2007)Munetoh, Motooka, Moriguchi, and Shintani]
- O–H [Ni et al.(2004)Ni, Lee, and Sinnott]
- O–C [Ni et al.(2004)Ni, Lee, and Sinnott]
- O–Si [Munetoh et al.(2007)Munetoh, Motooka, Moriguchi, and Shintani]
- O–Zn [Erhart et al.(2006)Erhart, Juslin, Goy, Nordlund, Müller, and Albe]
- O–Fe Byggmästar et al. Article in preparation, parameters available on request.
- O–Be Byggmästar et al. Article in preparation, parameters available on request.

Si–X

- Si–Si [Tersoff(1986)]
- Si–Si [Tersoff(1988c)]
- Si–Si [Tersoff(1988a)]
- Si–Si [Erhart and Albe(2005)]
- Si–O [Munetoh et al.(2007)Munetoh, Motooka, Moriguchi, and Shintani]
- Si–C [Erhart and Albe(2005)]

Cr–X

- Cr–Cr [Henriksson et al.(2013)Henriksson, Björkas, and Nordlund]
- Cr–Fe [Henriksson et al.(2013)Henriksson, Björkas, and Nordlund]
- Cr–C [Henriksson et al.(2013)Henriksson, Björkas, and Nordlund]

Fe–X

- Fe–Fe [Müller et al.(2007a)Müller, Erhart, and Albe]
- Fe–Cr [Henriksson et al.(2013)Henriksson, Björkas, and Nordlund]
- Fe–C [Henriksson et al.(2013)Henriksson, Björkas, and Nordlund]
- Fe–C [Henriksson and Nordlund(2009)]
- Fe–O Byggmästar et al. Article in preparation, parameters available on request.
- Fe–H [Kuopanportti et al.(2016)Kuopanportti, Hayward, Fu, Kuronen, and Nordlund]
- Fe–Pt [Müller et al.(2007b)Müller, Erhart, and Albe]

Zn– X

Zn–Zn [Erhart et al.(2006)Erhart, Juslin, Goy, Nordlund, Müller, and Albe]

Zn–O [Erhart et al.(2006)Erhart, Juslin, Goy, Nordlund, Müller, and Albe]

Ga– X

Ga–Ga [Albe et al.(2002b)Albe, Nordlund, Nord, and Kuronen]

Ga–As [Albe et al.(2002b)Albe, Nordlund, Nord, and Kuronen]

Ga–N [Nord et al.(2003)Nord, Albe, Erhart, and Nordlund]

Ge– X

Ge–Ge [Tersoff(1989)]

As– X

As–As [Albe et al.(2002b)Albe, Nordlund, Nord, and Kuronen]

As–Ga [Albe et al.(2002b)Albe, Nordlund, Nord, and Kuronen]

Y– X

Y–Y [Fan et al.(2013)Fan, Yang, Tang, Sun, Dai, Peng, Zhou, and Zu]

W– X

W–W [Juslin et al.(2005)Juslin, Erhart, Träskelin, Nord, Henriksson, Nordlund, Salonen, and Albe]

W–W [Ahlgren et al.(2010)Ahlgren, Heinola, Juslin, and Kuronen]

W–C [Juslin et al.(2005)Juslin, Erhart, Träskelin, Nord, Henriksson, Nordlund, Salonen, and Albe]

W–H [Juslin et al.(2005)Juslin, Erhart, Träskelin, Nord, Henriksson, Nordlund, Salonen, and Albe]

W–N [Polvi et al.(2016)Polvi, Heinola, and Nordlund]

W–Be [Björkas et al.(2010)Björkas, Henriksson, Probst, and Nordlund]

Pt– X

Pt–Pt [Albe et al.(2002a)Albe, Nordlund, and Averbäck]

Pt–C [Albe et al.(2002a)Albe, Nordlund, and Averbäck]

Pt–Fe [Müller et al.(2007b)Müller, Erhart, and Albe]

Au– X

Au–Au [Backman et al.(2012)Backman, Juslin, and Nordlund]

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