Table 4.1: Calculated bulk properties (equilibrium lattice constants[Å], bulk moduli[GPa]) Reference[a] "Transition metal carbides and nitrides"

Bulk	present work (Å)	Ref[a] (Å)	Deviation (%)
TiC(np)	4.35 220	4.33	+0.5
TiC(pc)	4.33 262		0.0
TaC(np)	4.42 330	4.46	0.9
TaC(pc)	4.46 342		0.0
HfC(np)	4.55 244	4.64	1.9
HfC(pc)	4.59 258		1.1
NbC(np)	4.44 320	4.47	0.7
NbC(pc)	4.48 312		+0.2
OsC(np)	4.51 310		
OsC(pc)	4.55 302		
ZrC(np)	4.62 242	4.70	1.7
ZrC(pc)	4.66 239		0.9