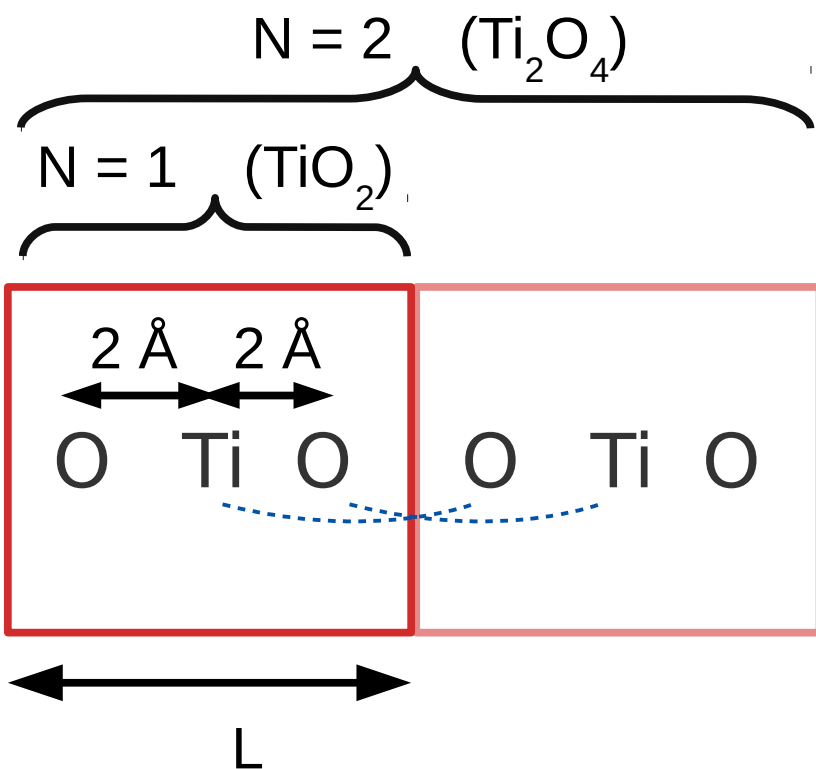


Linear TiO₂ chains -- DFTB+ versus CP2K

Cells sizes are (N*L x 5 Å x 5 Å)
Largest repulsion cutoff is 4.8 Å



L (Å)	N (-)	Repulsive Energy (Ha)		
		DFTB+	CP2K	Δ
25	1	0.0782189 756	0.078218 9206	~0
6	1	0.0782189 756	0.078218 9206	~0
5	1	0.4988475 818	0.493906 3549	0.00494 12269
5	2	0.9976951 635	0.997694 7534	~0

CP2K results not 'size-extensive', suggesting some interaction is missing in the (L=5, N=1) case. The |Δ| value is matched exactly by twice the repulsive energy between O and Ti at 3 Å (pairs with dashed blue lines). The cutoff for the O-Ti repulsion amounts to 3.39 Å.