Supplementary Materials For: Effective Wang-Teter Kernels for Orbital-Free DFT

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I. ADDITIONAL TABLES

	KIN	ENE	DEN	AVE
β-tin	3.49169	3.51565	3.65791	3.86712
BCC	5.62952	5.64018	5.69329	6.00582
FCC	4.79818	4.82134	4.49756	4.01807
HCP	2.17497	2.29267	2.2831	2.96179
BCT5	2.21286	2.34529	2.63874	3.01834
SH	4.20006	4.21712	4.33257	4.27526
CD	2.79672	2.88202	4.69511	3.50586
DHCP	3.61805	3.63498	3.75672	3.38523

TABLE S1. Parameter ρ_0 in Hartree atomic units for the equilibrium structure of all Si phases considered. All values should be multiplied by 10^{-2}.

	KIN	ENE	DEN	AVE	KS
β-tin	1.379	1.374	1.343	1.298	1.287
BCC	2.346	2.337	2.401	2.415	1.835
FCC	1.109	1.108	1.109	1.103	0.990
HCP	2.234	2.233	2.214	2.250	2.190
BCT5	1.270	1.251	1.235	1.143	1.291
SH	5.531	5.514	5.412	5.146	6.706
CD	0.533	0.518	0.516	0.457	1.542
DHCP	1.099	1.076	1.022	0.968	3.998

TABLE S2. Values of H_f for the lesser Fukui function, f_-, evaluated by KS-DFT and OF-DFT. $H_f = \int \frac{(f_-(\mathbf{r})-1)(f_-(\mathbf{r}')-1)}{|\mathbf{r}-\mathbf{r}'|} d\mathbf{r}$.

	KIN	ENE	DEN	AVE	KS
β-tin	32.215	32.209	32.113	32.038	31.994
BCC	50.591	50.546	51.077	52.413	55.799
FCC	33.804	33.814	33.752	33.547	33.876
HCP	21.127	21.080	20.896	20.925	21.697
BCT5	54.512	54.521	54.760	53.099	51.507
SH	23.435	24.597	24.860	24.122	22.399
CD	32.488	32.379	32.388	31.946	29.052
DHCP	58.821	58.200	56.875	55.513	52.799

TABLE S3. Low-q total electronic energy response ($n_a = 1$ in Eq. (15)). The reported values measure the departure of the response energy from the ground state energy, $\frac{E[n_{\text{resp}}]-E[n]}{A}$ in meV/atom.

	KIN	ENE	DEN	AVE	KS
β-tin	15.393	15.378	15.382	15.406	15.225
BCC	5.841	5.839	5.841	5.839	5.828
FCC	7.269	7.269	7.269	7.270	7.261
HCP	5.325	5.345	5.325	5.336	4.938
BCT5	6.848	6.848	6.848	6.844	6.833
SH	5.693	5.247	5.266	5.653	5.0183
CD	20.219	20.213	20.222	20.210	19.987
DHCP	8.697	8.686	8.683	8.674	8.609

TABLE S4. High-q total electronic energy response ($n_a = 5$ in Eq. (15)). The reported values measure the departure of the response energy from the ground state energy, $\frac{E[n_{\text{resp}}]-E[n]}{A}$ in meV/atom.

	KIN	ENE	DEN	AVE	KS
β-tin	8.982	14.865	9.851	9.303	6.934
BCC	29.136	29.125	28.498	29.349	40.987
FCC	15.763	15.768	15.727	14.888	20.558
HCP	183.762	182.685	181.938	182.836	193.871
BCT5	24.311	24.309	24.247	24.517	24.372
SH	-462.603	-400.536	-469.994	-468.439	-435.262
CD	6.309	6.540	6.532	6.818	5.487
DHCP	53.859	54.745	56.321	57.686	51.096

TABLE S5. Low-q noninteracting kinetic energy response ($n_a = 1$ in Eq. (15)). The reported values measure the departure of the response energy from the ground state energy, $\frac{T_s[n_{\rm resp}]-T_s[n]}{A}$ in meV/atom.

	KIN	ENE	DEN	AVE	KS
β-tin	16.370	21.988	17.159	16.542	15.761
BCC	6.593	6.682	7.447	6.962	5.788
FCC	8.173	8.177	8.150	7.272	7.272
HCP	-22.447	-24.286	-23.439	-23.301	-25.045
BCT5	7.151	7.151	7.155	7.018	7.314
SH	4.405	78.230	-23.269	-15.465	-5.649
CD	22.138	22.295	22.299	22.252	21.373
DHCP	10.193	10.402	10.345	9.833	8.625

TABLE S6. High-q noninteracting kinetic energy response ($n_a = 5$ in Eq. (15)). The reported values measure the departure of the response energy from the ground state energy, $\frac{T_s[n_{\rm resp}]-T_s[n]}{A}$ in meV/atom.

Functional	$T_{TF}[n] + T_{NL}[n]$
KIN	0
DEN	-0.651
ENE	-0.638
LMGP	0.216
LKT	1.636

TABLE S7. Helium atom test. For a two-electron system the vW potential is the exact noninteracting kinetic energy potential. Therefore, TF and the nonlocal parts of the energy ($T_{TF}[n] = -T_{NL}[n]$) and potential ($v_{TF}(\mathbf{r}) = -v_{NL}(\mathbf{r})$) should cancel out.