Name	E NIST	E pred	$|\Delta E|$	$|\Delta E|$/E NIST
Ecoul	1.9961	1.9963	0.0001	0.0001
Etot	-2.8348	-2.8348	0.0000	-0.0000
Exc	-0.9733	-0.9735	0.0002	-0.0002
Ekin	2.7679	2.7689	0.0010	0.0004
1s	-0.5704	-0.5728	0.0023	-0.0041

Orbital 1s eigen energy -0.5728