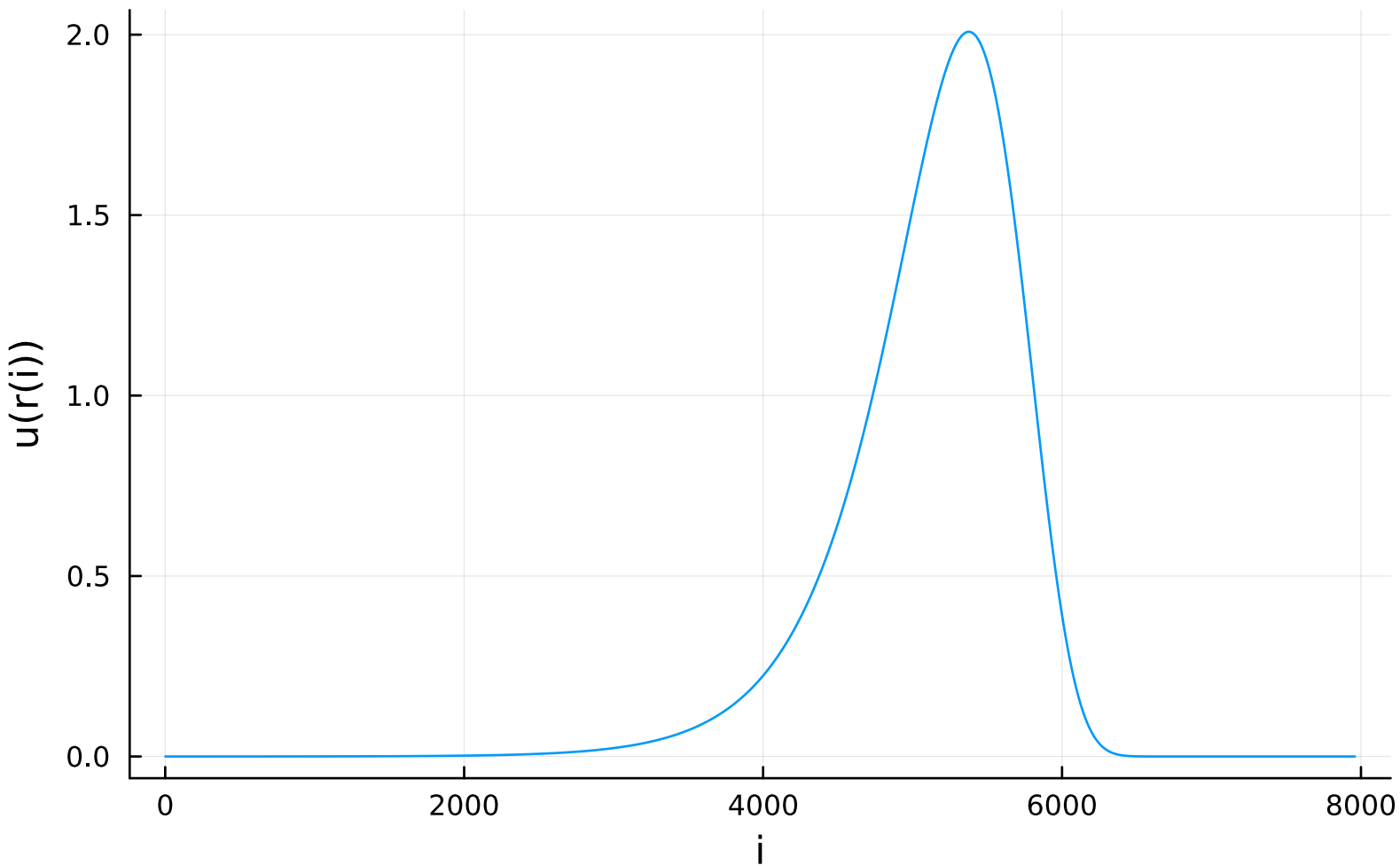
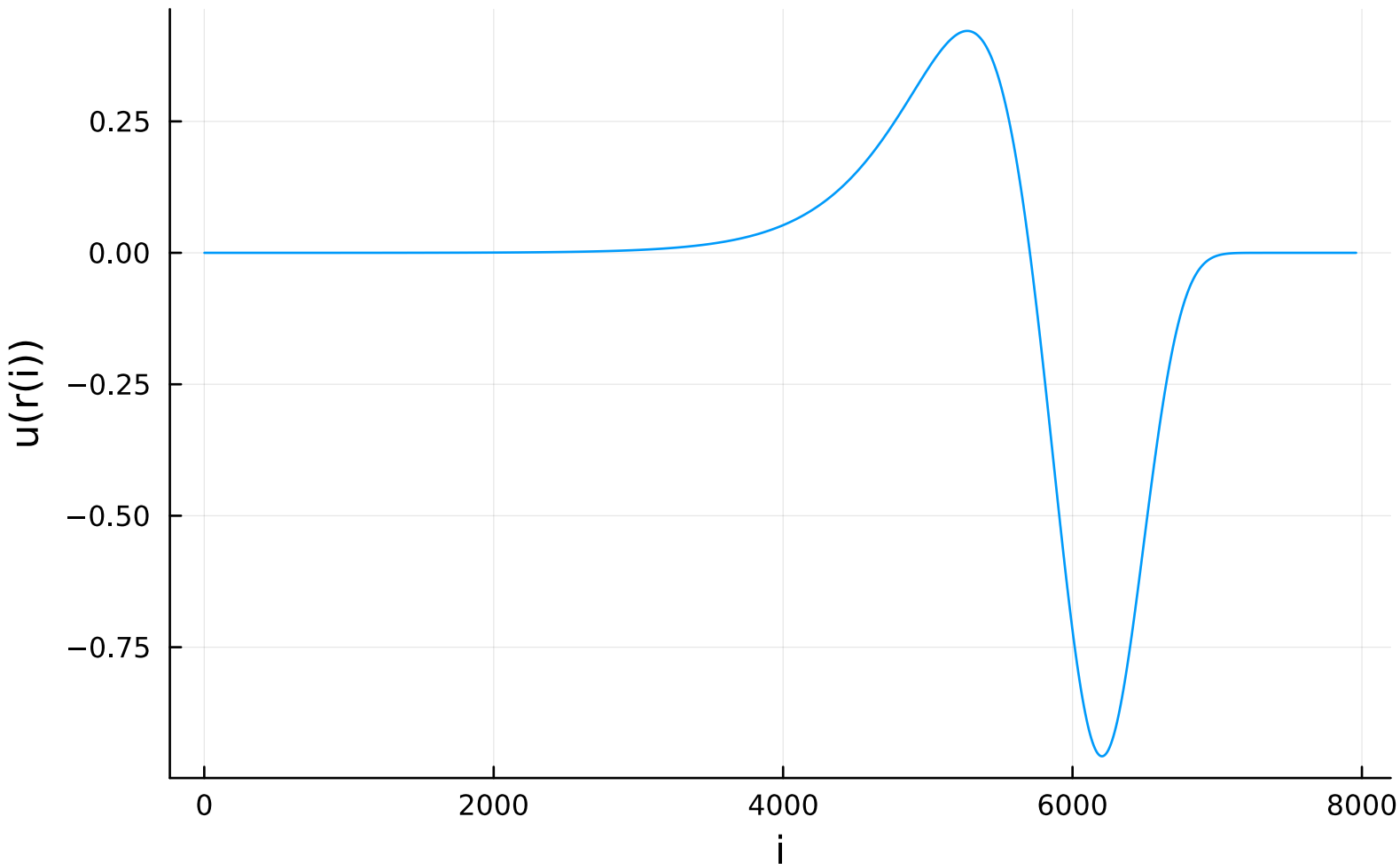


| | | | | |
|--------|--------------|------------|--------------|---------------------|
| Oxygen | E in Hartree | | | |
| Name | E NIST | E pred | $ \Delta E $ | $ \Delta E /E$ NIST |
| Ecoul | 36.331102 | 36.327422 | 0.003680 | 0.000101 |
| Etot | -74.473077 | -74.473077 | 0.000000 | -0.000000 |
| 2s | -0.871362 | -0.871820 | 0.000458 | -0.000526 |
| Exc | -7.768482 | -7.768109 | 0.000373 | -0.000048 |
| Ekin | 74.116881 | 74.112326 | 0.004555 | 0.000061 |
| 2p | -0.338381 | -0.338826 | 0.000445 | -0.001315 |
| 1s | -18.758245 | -18.758906 | 0.000661 | -0.000035 |

Orbital 1s eigen energy -18.7589



Orbital 2s eigen energy -0.8718



Orbital 2p eigen energy -0.3388

