A few molecular orbitals of H₂O (HF/3-21G*)

HOMO – 3
$E = -1.321$ au

HOMO – 2
$E = -0.68563$
A few molecular orbitals of H₂O (HF/3-21G*)

HOMO – 1

$E = -0.52980$

HOMO

$E = -0.4772$
A few molecular orbitals of H₂O (HF/3-21G*)

LUMO
\[ E = +0.2611 \]

LUMO + 1
\[ E = +0.3604 \]