Fig. 4. The local density of states projected onto an adsorbate state interacting with the \(d\) bands at a surface. The strength of the adsorbate–surface coupling matrix element \(V\) is kept fixed as the center of the \(d\) bands \(\epsilon_d\) is shifted up toward the Fermi energy \((\epsilon_F = 0)\) and the width \(W\) of the \(d\) bands is decreased to keep the number of electrons in the bands constant. As \(\epsilon_d\) shifts up, the antibonding states are emptied above \(\epsilon_F\) and the bond becomes stronger (bottom). The calculation was done by using the Newns–Anderson model (37). Adapted from Hammer (38).