Electronic Supplementary Material (ESI) for RSC Advances.

Accurate potential energy surfaces for the first two lowest electronic states of Li (2p) + H_2 reaction

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Attachment files

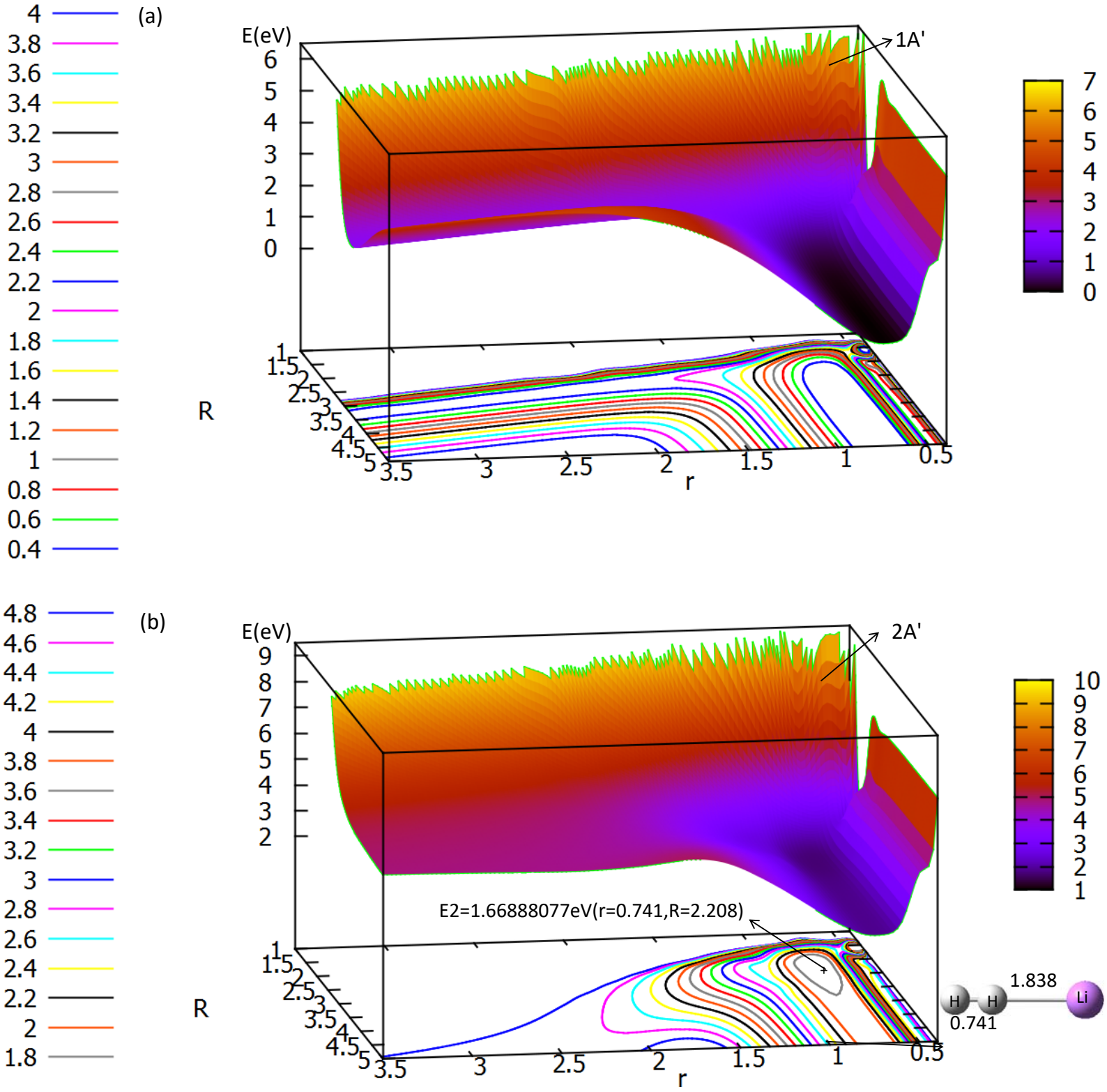

Figure 1A: Separated plotting the ground state (1A') and the first execited state (2A') PESs at θ=0° in Jacobi coordinate.

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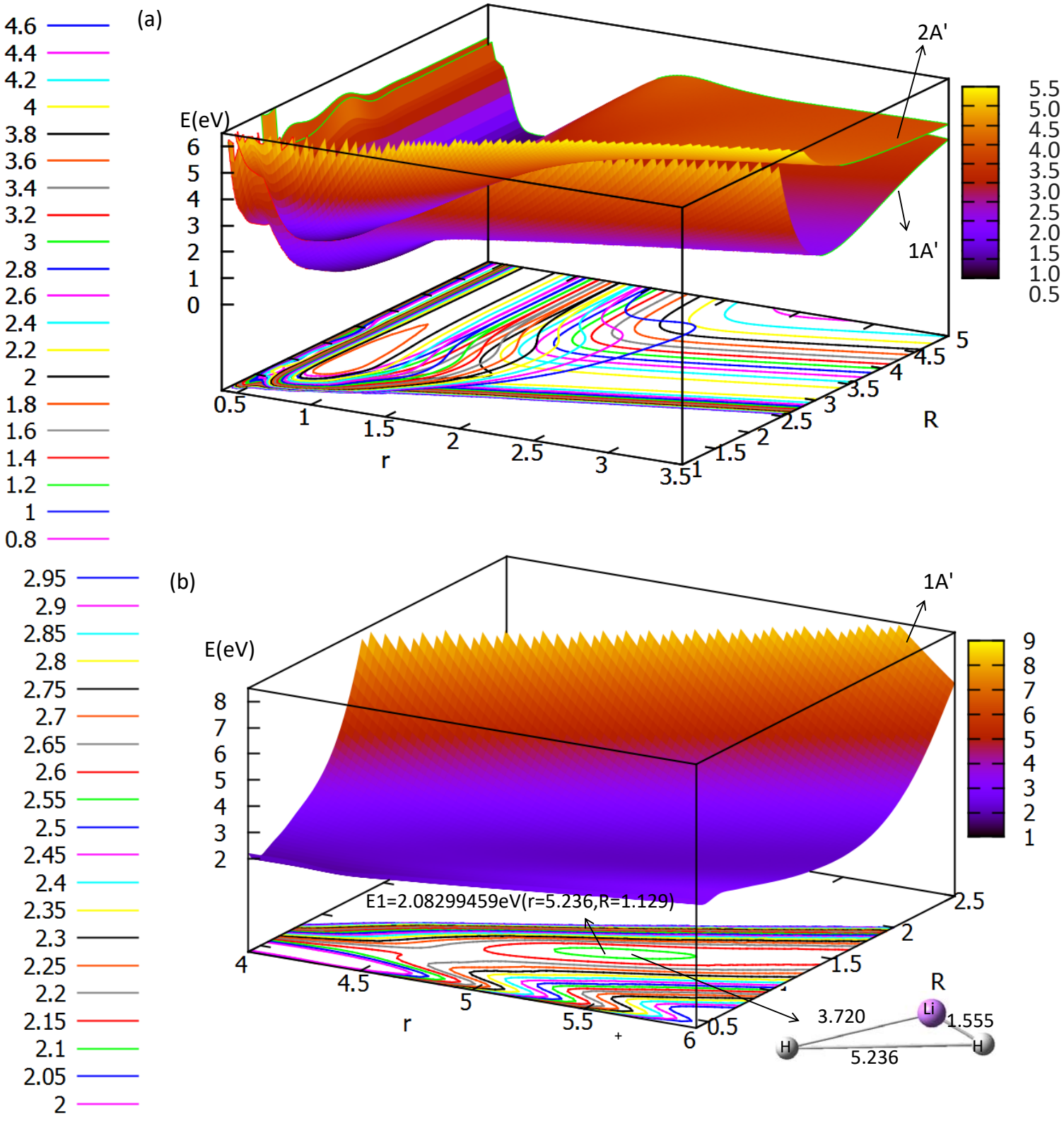

Figure 2A: Two potential energy surfaces (in eV) and contour plots of the potential energy surface as a function of distances r and R (in Å) at θ=15°.

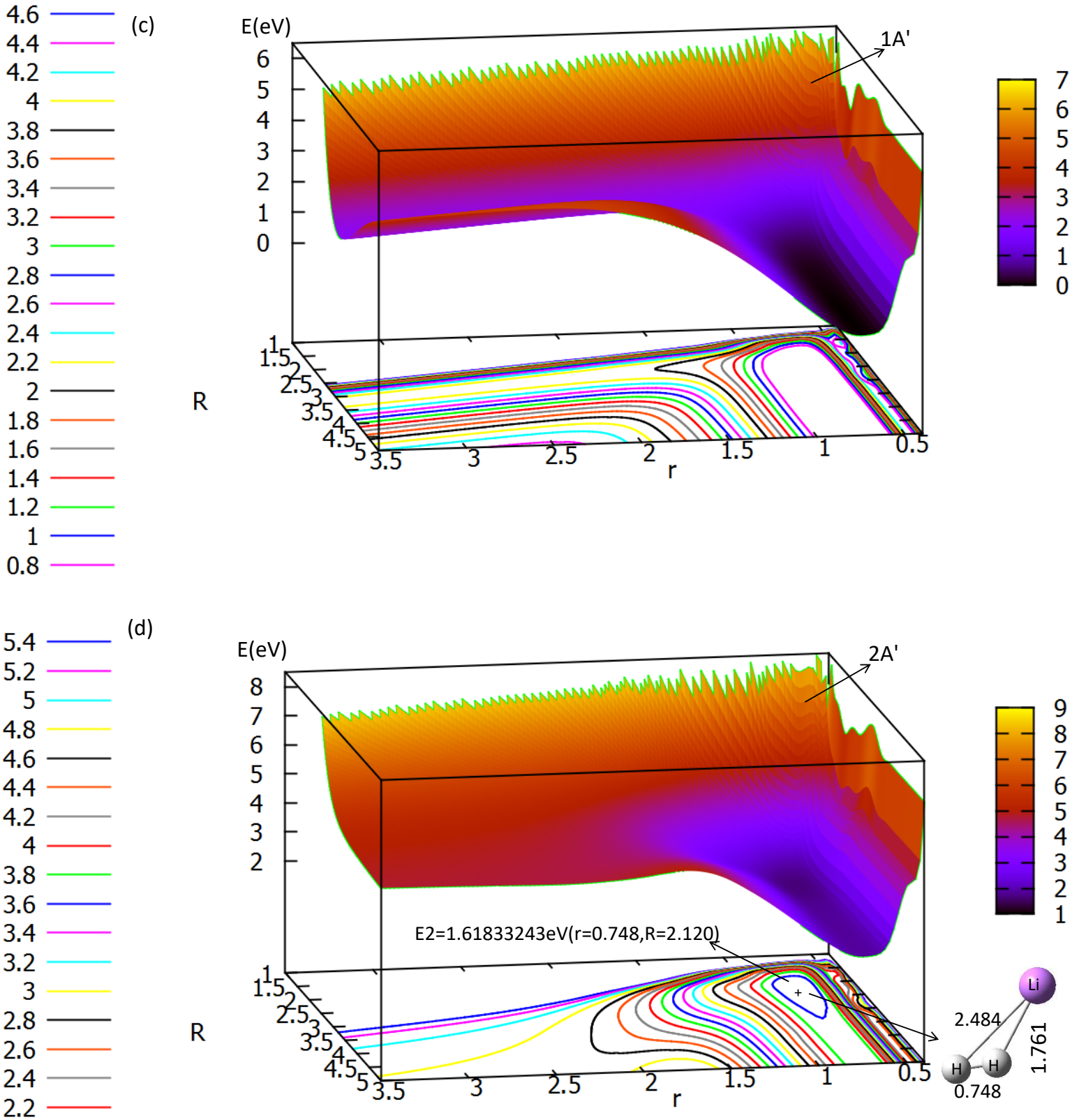

Figure 3A: Separated plotting the ground state (1A') and the first execited state (2A') PESs at θ=15° in Jacobi coordinate.

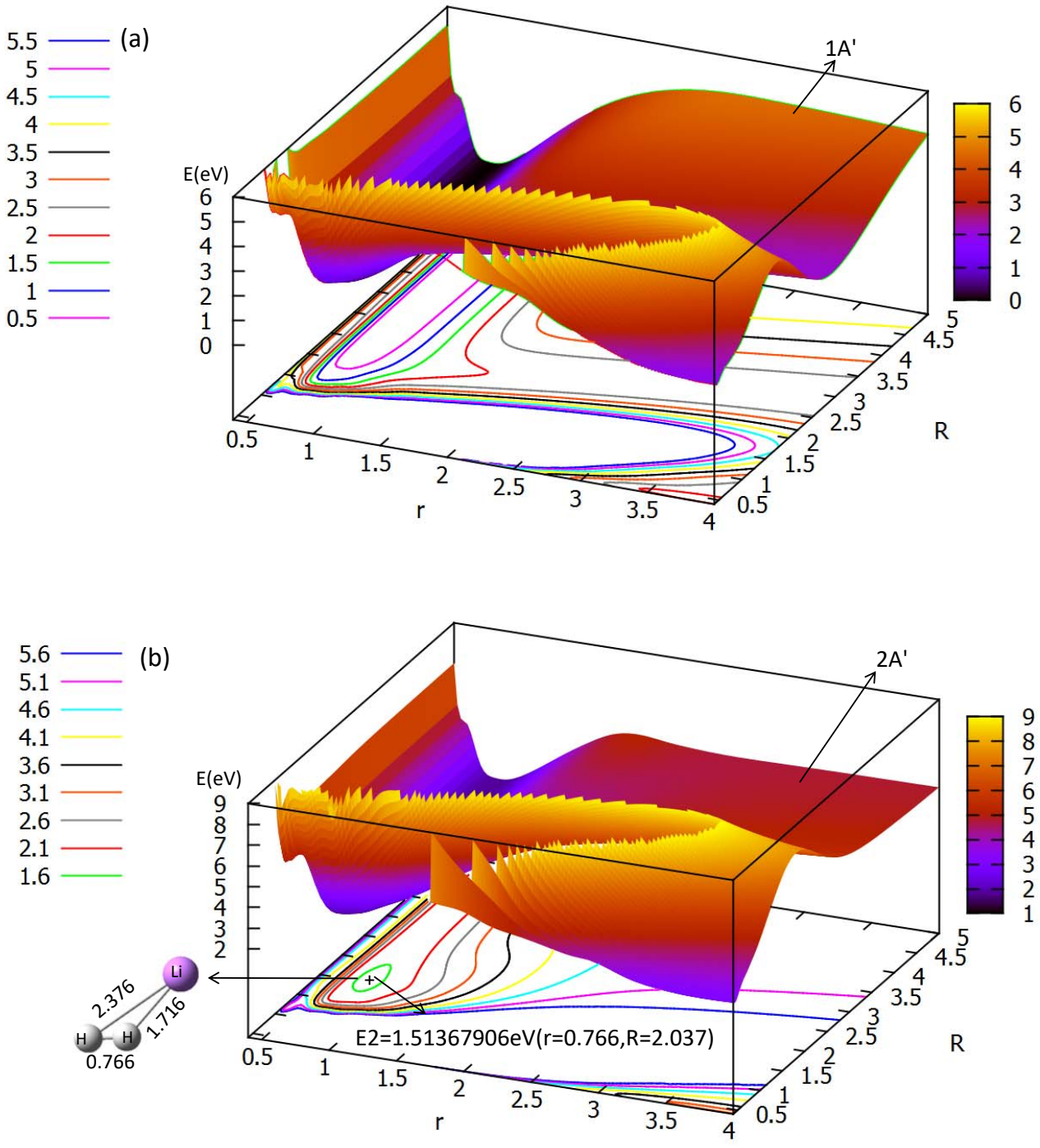

Figure 4A: Separated plotting the ground state (1A') and the first execited state (2A') PESs at θ=30° in Jacobi coordinate.

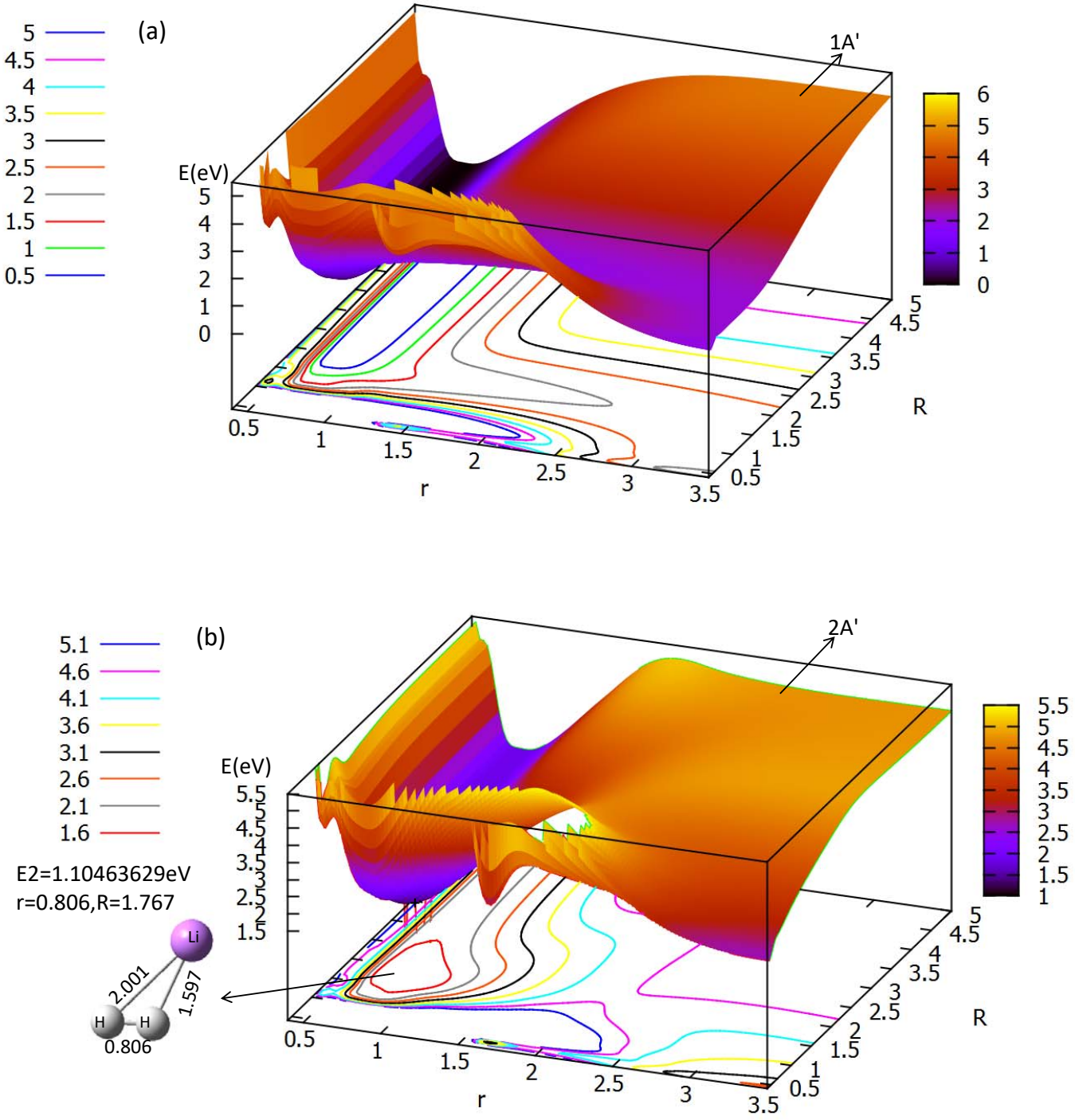

Figure 5A: Separated plotting the ground state (1A') and the first execited state (2A') PESs at θ=60° in Jacobi coordinate.

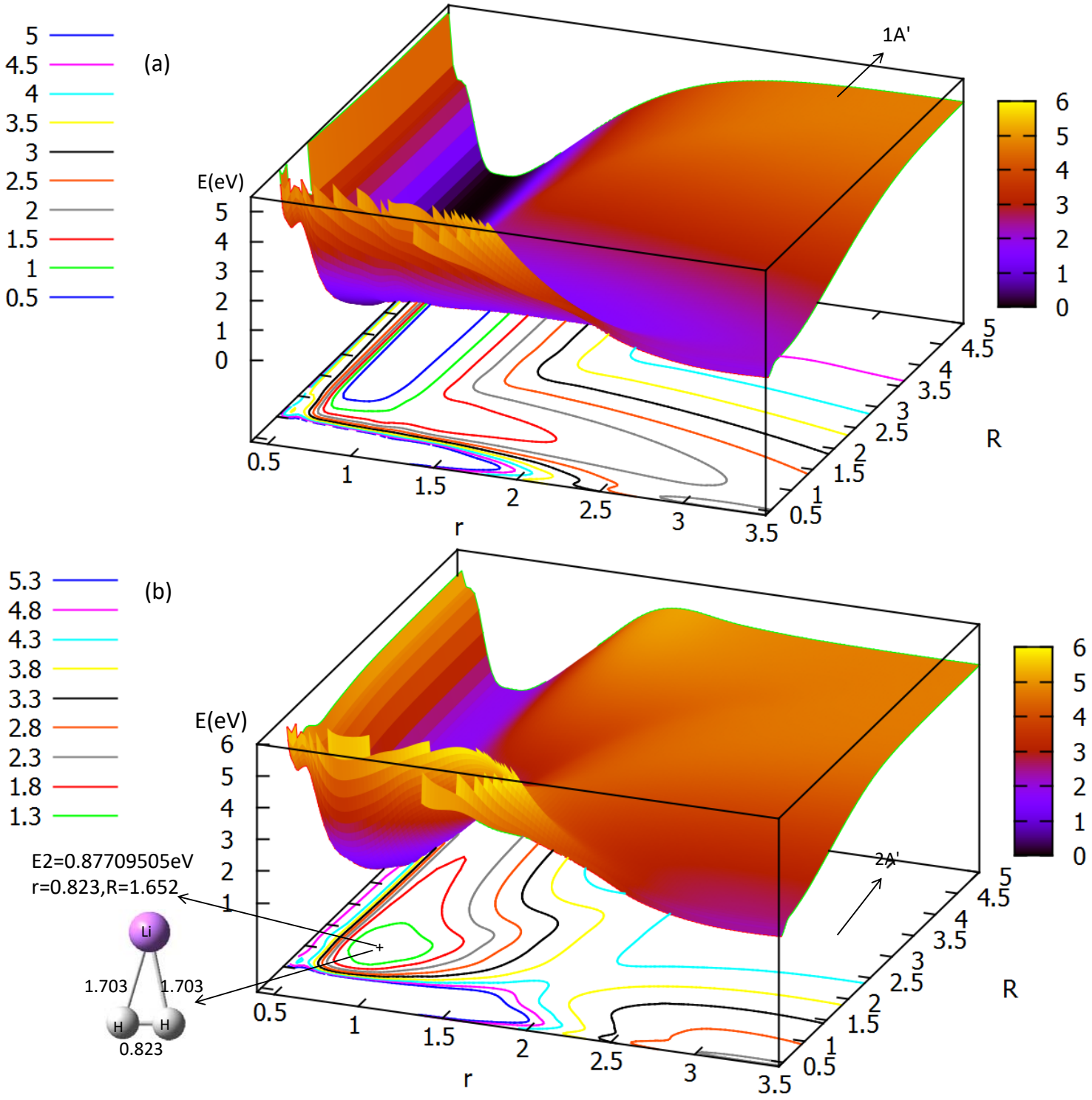

Figure 6A: Separated plotting the ground state (1A') and the first execited state (2A') PESs at θ=90° in Jacobi coordinate.