

### Aspirin - Deformation Density (blue=accumulation, red=depletion)

z=-0.7 Å

z=-0.7 Å

z=-0.5 Å

z=-0.3 Å

z=-0.3 Å



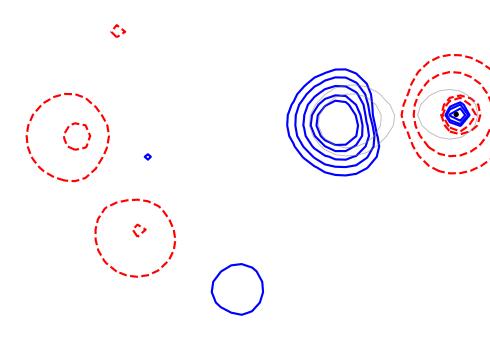
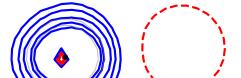
z=-0.1 Å

z=0.1 Å

z=0.1 Å

z=0.3 Å

z=0.6 Å



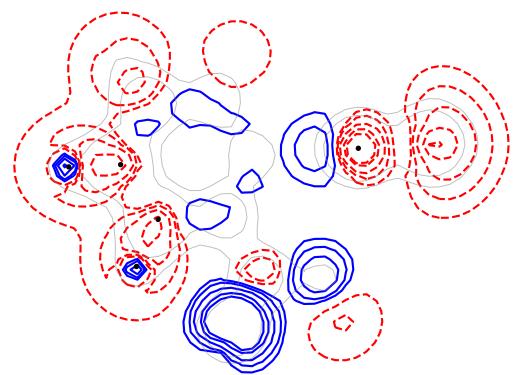
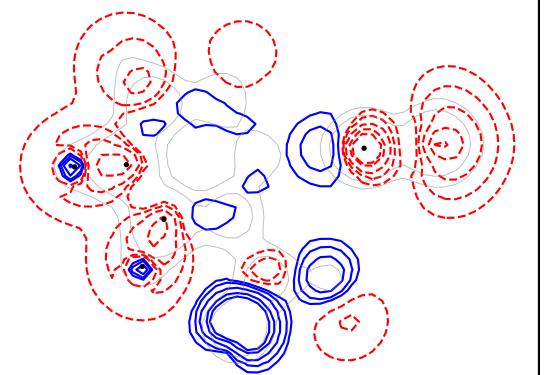
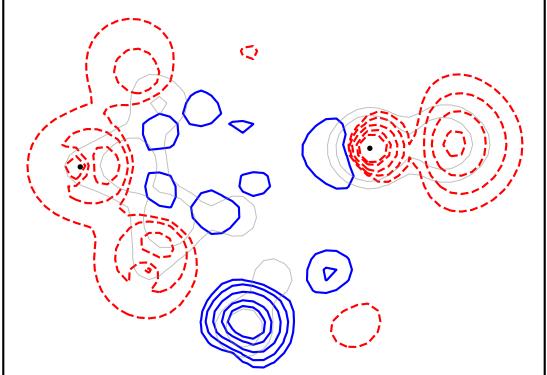
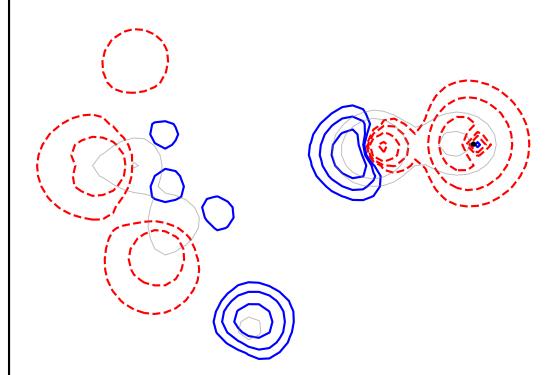
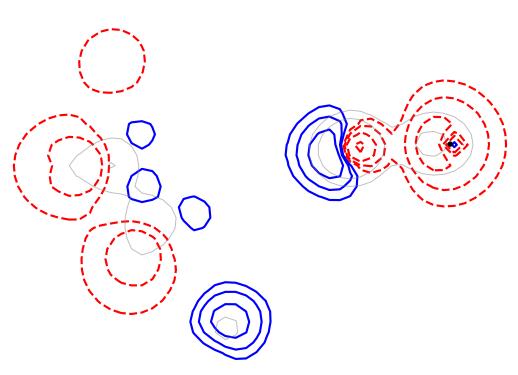
z=0.8 Å

z=0.8 Å

z=1.0 Å

z=1.2 Å

z=1.2 Å



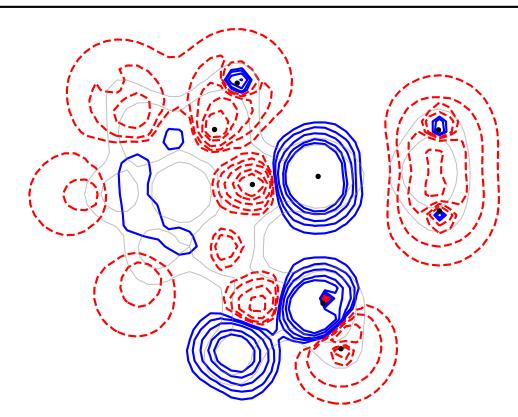
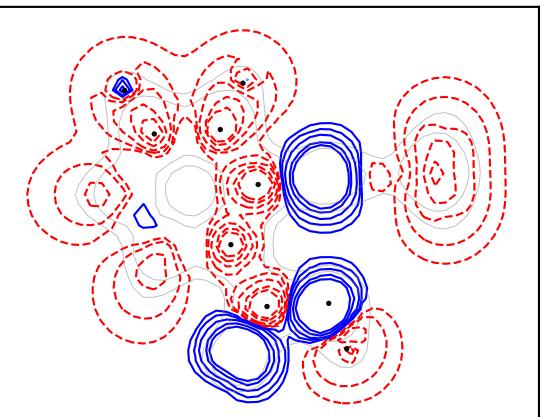
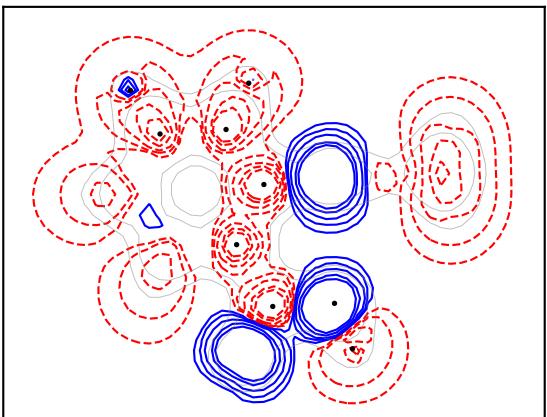
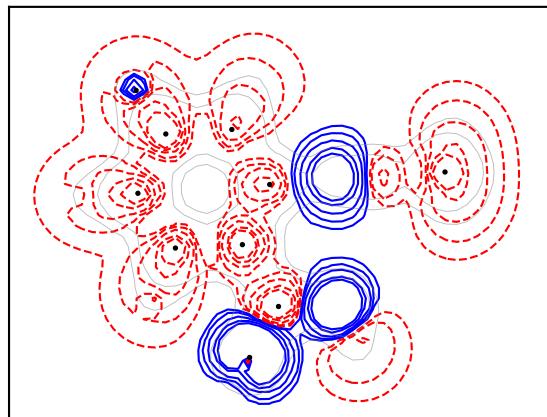
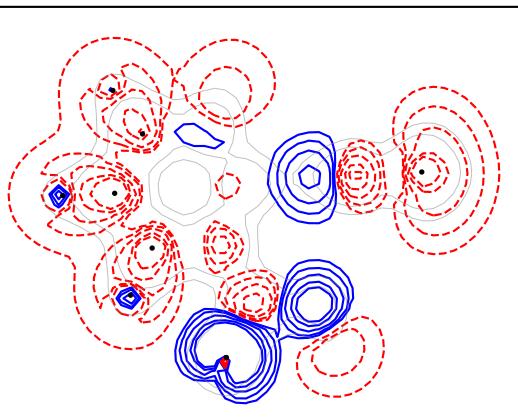
z=1.4 Å

z=1.6 Å

z=1.8 Å

z=1.8 Å

z=2.1 Å



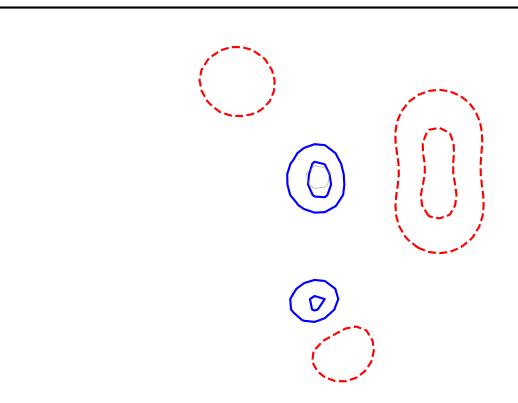
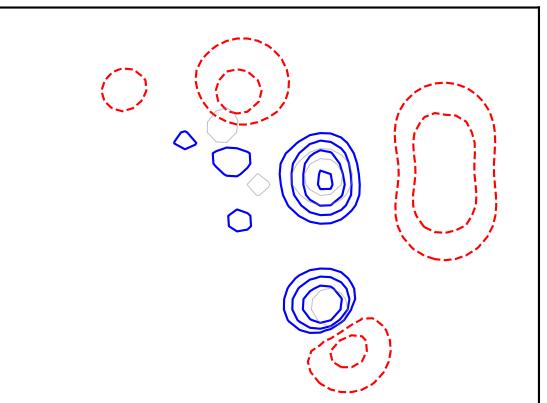
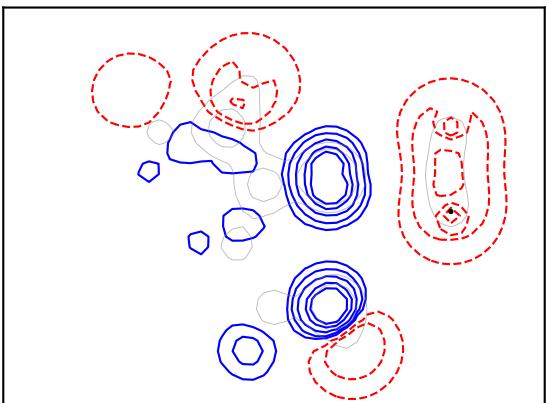
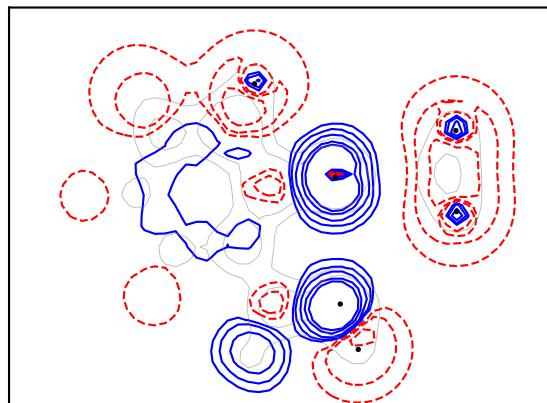
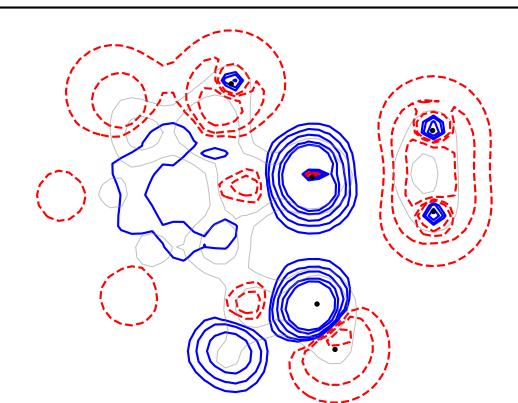
z=2.3 Å

z=2.3 Å

z=2.5 Å

z=2.7 Å

z=2.9 Å



### Aspirin - xTB Molecular Density (capped at 0.3)

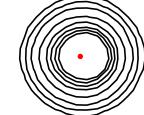
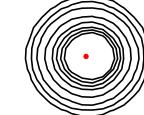
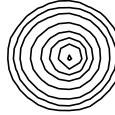
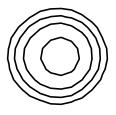
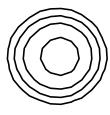
$z=-0.7\text{\AA}$  max=0.08

$z=-0.7\text{\AA}$  max=0.08

$z=-0.5\text{\AA}$  max=0.26

$z=-0.3\text{\AA}$  max=0.61

$z=-0.3\text{\AA}$  max=0.61



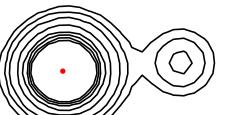
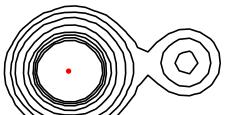
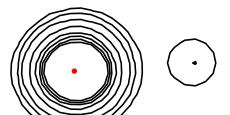
$z=-0.1\text{\AA}$  max=0.95

$z=0.1\text{\AA}$  max=1.21

$z=0.1\text{\AA}$  max=1.21

$z=0.3\text{\AA}$  max=1.03

$z=0.6\text{\AA}$  max=0.51



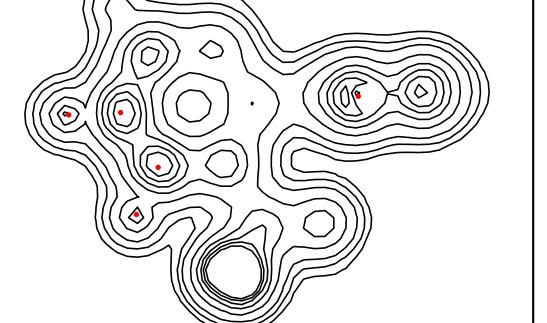
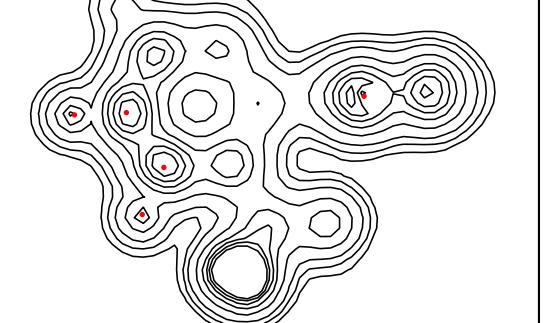
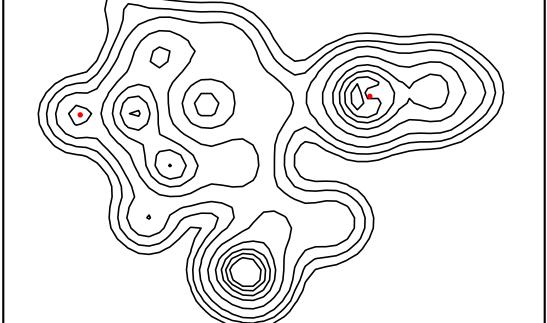
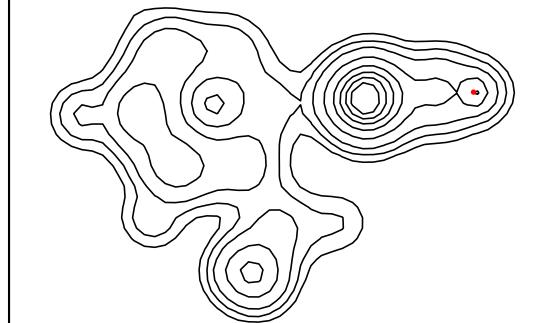
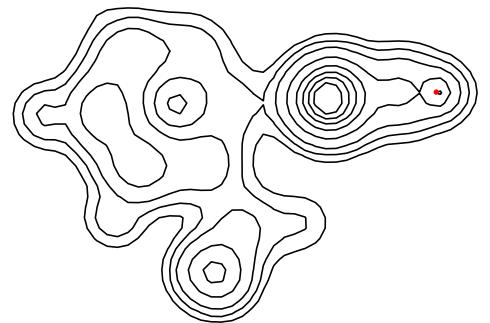
$z=0.8\text{\AA}$  max=0.32

$z=0.8\text{\AA}$  max=0.32

$z=1.0\text{\AA}$  max=0.37

$z=1.2\text{\AA}$  max=0.84

$z=1.2\text{\AA}$  max=0.84



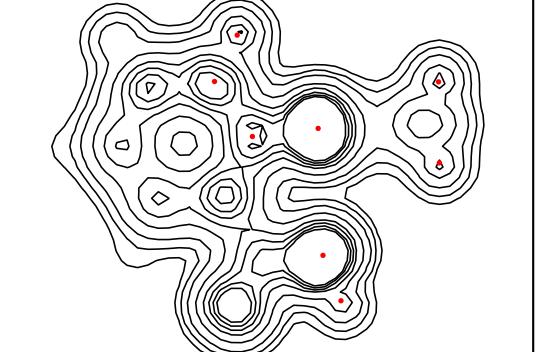
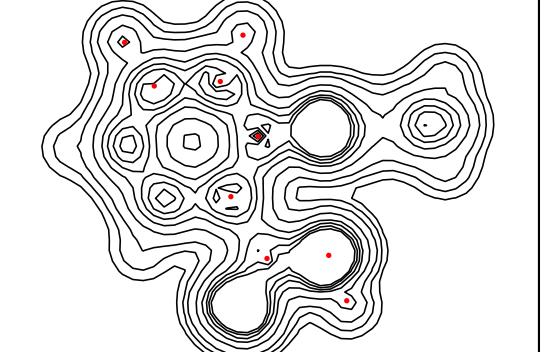
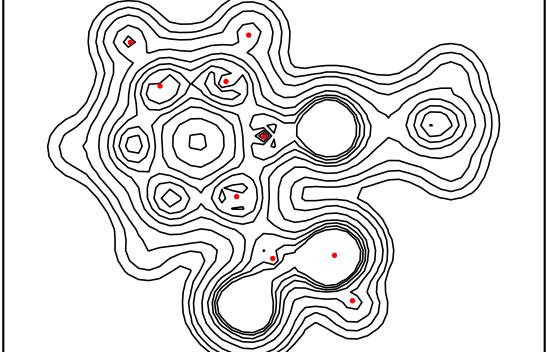
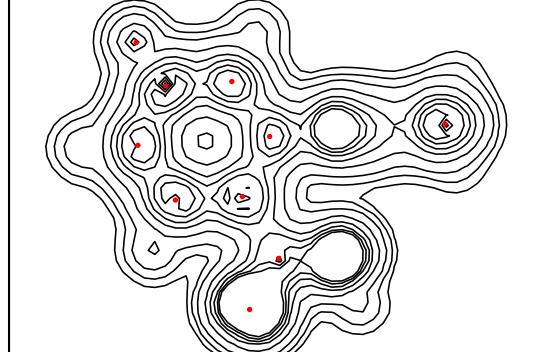
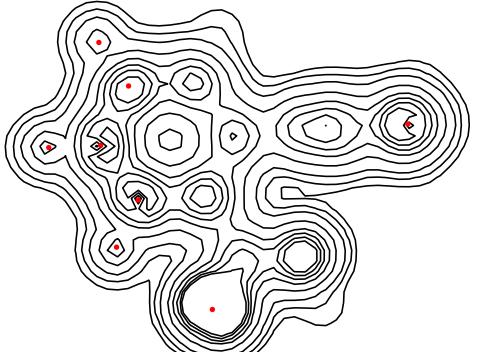
$z=1.4\text{\AA}$  max=1.18

$z=1.6\text{\AA}$  max=1.20

$z=1.8\text{\AA}$  max=1.24

$z=1.8\text{\AA}$  max=1.24

$z=2.1\text{\AA}$  max=1.24



$z=2.3\text{\AA}$  max=0.95

$z=2.3\text{\AA}$  max=0.95

$z=2.5\text{\AA}$  max=0.56

$z=2.7\text{\AA}$  max=0.26

$z=2.9\text{\AA}$  max=0.08

