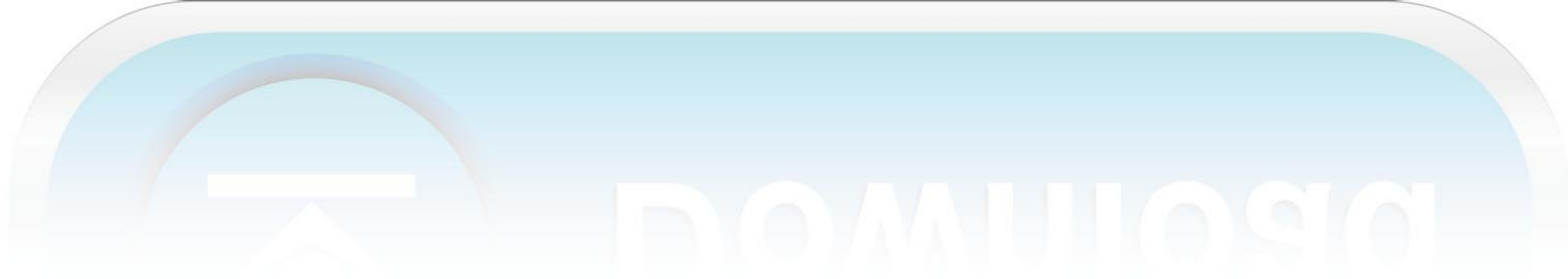




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Major New Features:

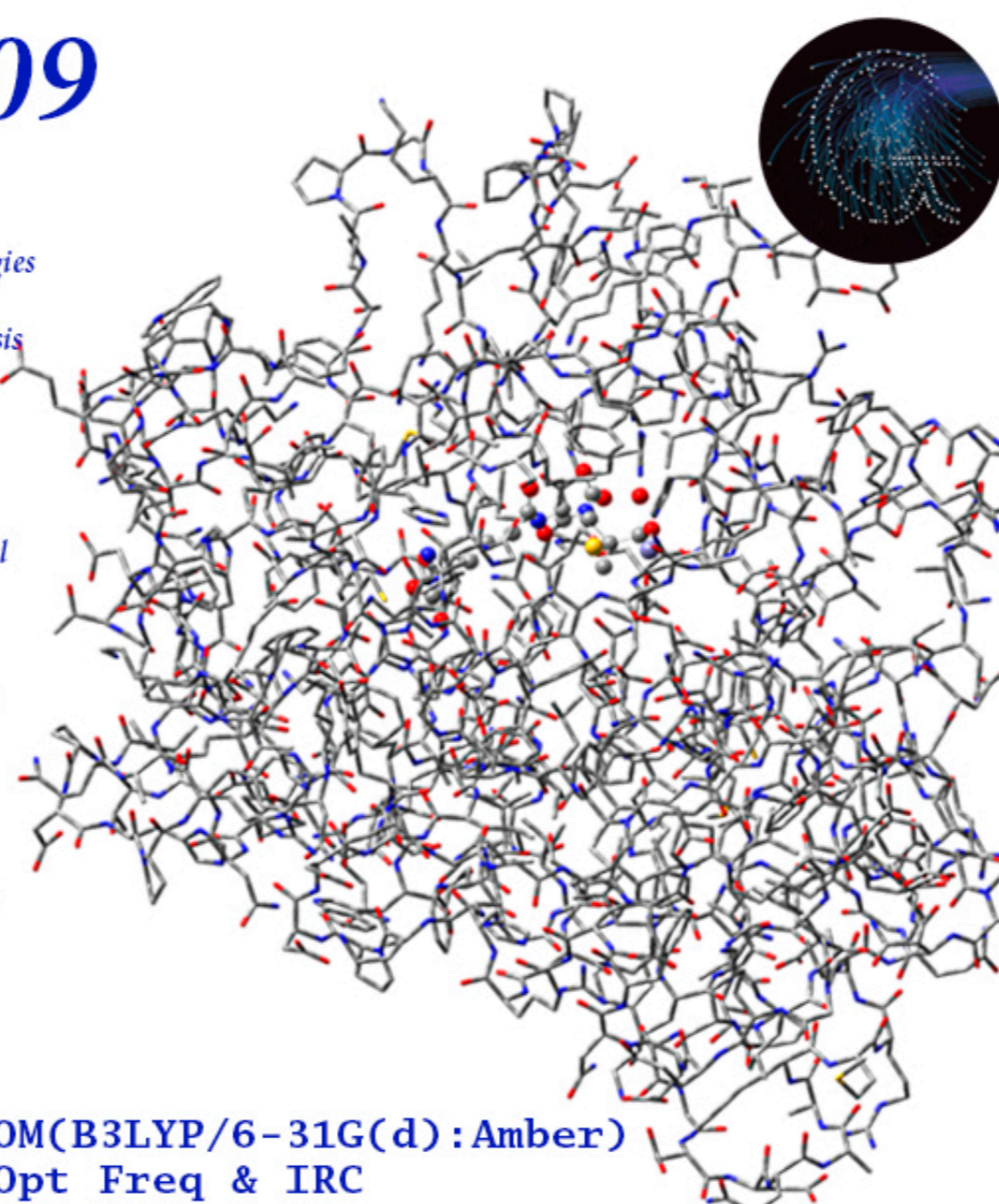
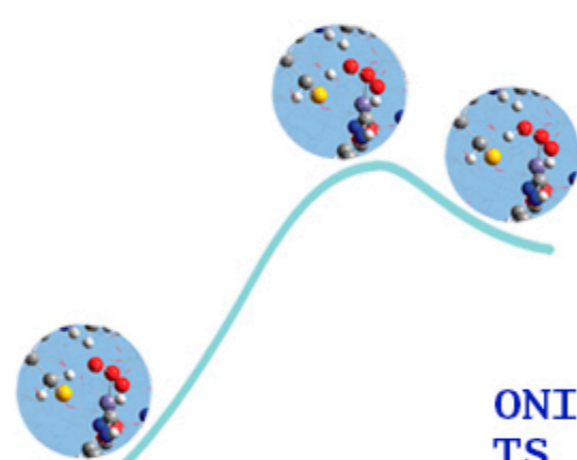
- ◆ ONIOM IRC & frequencies
- ◆ TD-DFT optimizations, EOMCC energies
- ◆ IEFPCM solvation for all properties
- ◆ Anharmonic frequencies, FCHT analysis

Performance Enhancements:

- ◆ Optimizations for large molecules
- ◆ New IRC algorithm
- ◆ Large frequency calculations in parallel

Challenging Calculation:

- ◆ Isopenicillin N synthase reaction paths

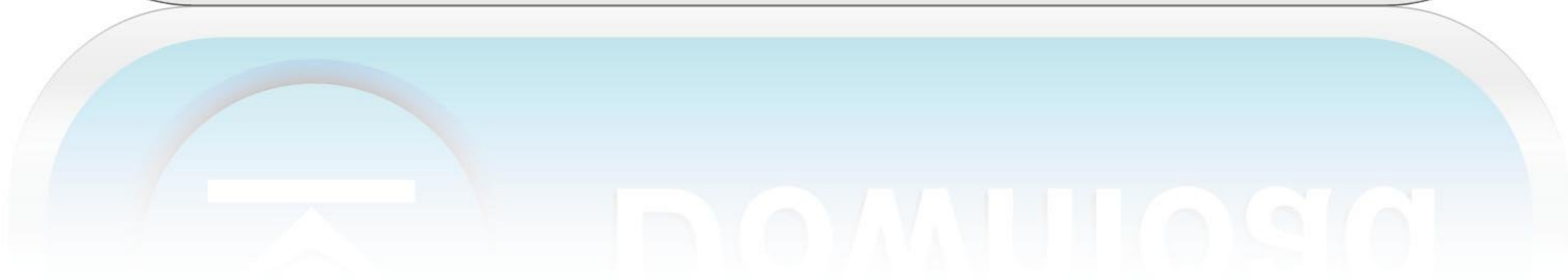


ONIOM(B3LYP/6-31G(d):Amber)
TS Opt Freq & IRC

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