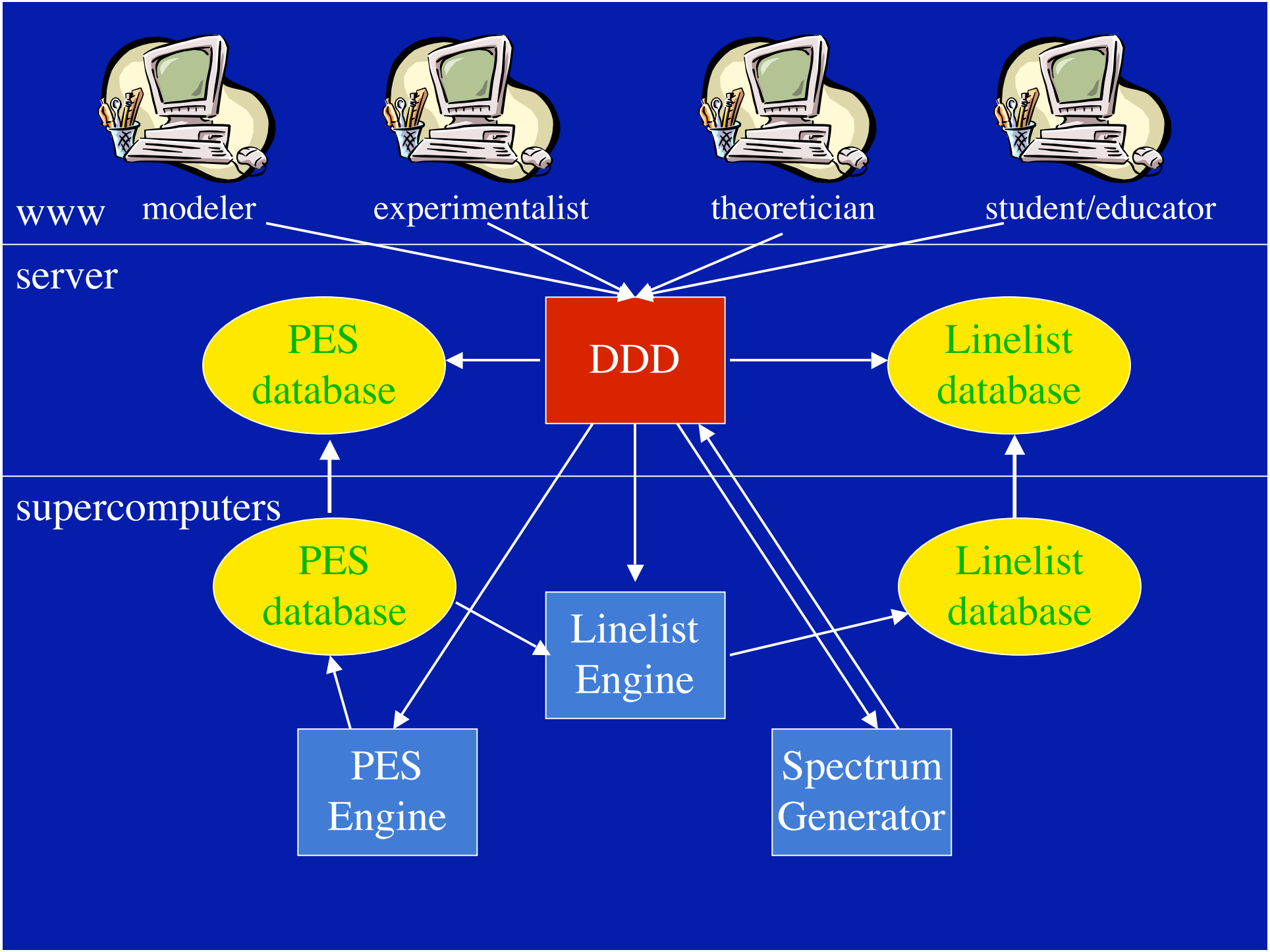
High accuracy spectroscopic data from calculations

David W. Schwenke

TNA

Diatomic data requests

- Thermal Protection
  - CN, N_2, NO,…
- Brown dwarfs
  - CrH, FeH, MgH, CaH, KCl, CsCl, NaCl, RbCl, LiCl, CaCl,…
- Stars
  - TiO, VO, ZrO, LaO, ScO, YO, AlO, AlH, LiH, CS, CH, C_2, NH, OH, SiO, MgH,…


www
modeler
experimentalist
theoretician
student/educator
server
PES database
DDD
Linelist database
supercomputers
PES database
Linelist Engine
Linelist database
PES Engine
Spectrum Generator

Summary of electronic states for C N

	$T_e(cm^{-1})$	ω_e	B_e	A_r
$^4\Sigma^+$	67917.36	1073.	1.316	
$^2\Pi_r$	67620.39	1351.	1.174	29.
$^4\Pi_r$	66585.79	2393.	1.714	48.
$^2\Delta_r$	60704.62 (60096)	1549. (1239)	1.375(1.383)	47.(29)
$^2\Sigma^-$	59638.83	1242.	1.347	
$^2\Sigma^+$	59439.56 (59151)	1721. (1681)	1.456(1.4871)	
$^2\Phi_r$	59291.08	931.	1.095	15.
$^2\Pi_r$	58747.56	2187.	1.429	5.
$^4\Sigma^-$	52655.15	1260.	1.348	
$^2\Pi_r$	51761.07 (54486)	1133. (1004)	1.045(1.162)	59.(-3)
$^4\Delta_r$	46864.38	1309.	1.367	1.
$^4\Pi_r$	44243.48	923.	1.104	47.
$^4\Sigma^+$	36466.04	1326.	1.367	
$^2\Sigma^+$	27128.65 (25752)	2059. (2163)	1.868(1.973)	
$^2\Pi_i$	8401.73 (9245)	1766. (1812)	1.642(1.7151)	-49.(-53)
$^2\Sigma^+$	0.00	2028.(2068)	1.818(1.8997)	

Summary of electronic states for TiO

	Te(1/cm)	we	Be
5SIGMA-	42905.21	672.	0.389
5DELTA	39146.58	619.	0.378
5PI	37889.33	649.	0.361
5PI	35483.44	916.	0.368
5PHI	35046.40	656.	0.350
5PI	34784.87	476.	0.392
1DELTA	34354.62	1476.	0.332
3DELTA	33721.58	418.	0.418
5SIGMA-	32646.85	844.	0.408
3PI	32222.75	2224.	0.497
5PHI	32153.63	669.	0.401
5DELTA	30382.19	616.	0.362
5SIGMA+	30119.22	620.	0.364
5SIGMA-	30042.09	652.	0.367
1PHI	29400.26	834.	0.402
3DELTA	28625.02	3151.	0.329
1PI	27939.92	2472.	0.334
3PI	27704.47	2564.	0.462
5PI	27667.58	629.	0.381
5GAMMA	27402.06	636.	0.369
1SIGMA+	27248.60	968.	0.507
5DELTA	26300.93	651.	0.375
3PHI	26294.02	2798.	0.406
1GAMMA	24446.94	963.	0.506
1PI	19573.49	946.	0.500
3SIGMA-	18778.67	979.	0.501
3PI	16990.68	878.	0.491
1SIGMA+	9422.57	1028.	0.543
1DELTA	4511.08	1061.	0.540
3DELTA	0.00	1099.	0.535

H_2O

- The most extensively studied molecule
- Partridge and Schwenke, 1996
  - *ab initio* calculations + empirical refinements lead to 0.05 cm^{-1} accuracy
- O. L. Polyansky, A. G. Császár, S. V. Shirin, N. F. Zobov, P. Barletta, J. Tennyson, D. W. Schwenke, and P. J. Knowles, Science 2003
  - Purely *ab initio* calculations. All known band origins are predicted within 0.75 cm^{-1}

CH_4

- Above 6000 cm^{-1} experimental spectrum is too congested to analyze
- High symmetry, symmetric top
- 9 vibrational coordinates
- PES based on *ab initio* calculations at 8267 geometries

2/2 Results