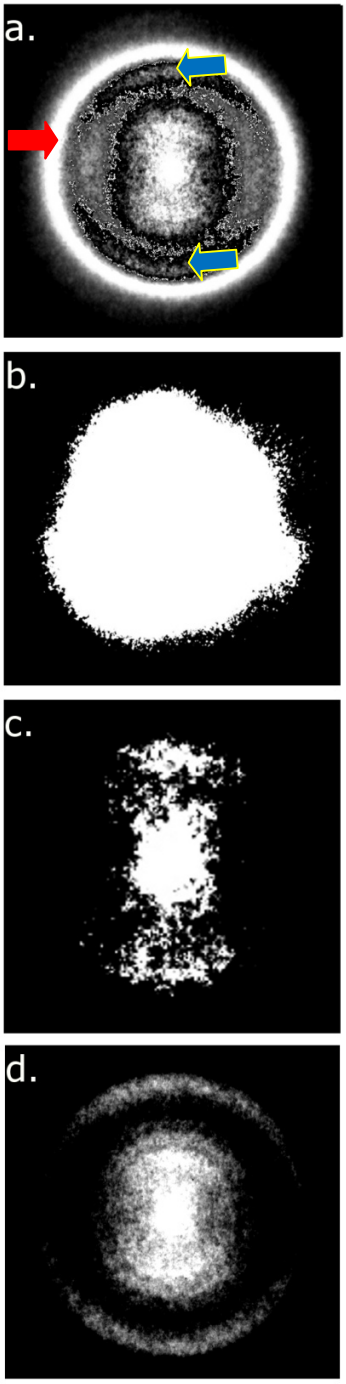
Supplemental Material



Supporting Figure 1. This figure displays steps in the image extraction process for NbSi. Image **a.** shows the raw $NbSi^-$ photoelectron image. The Red arrow depicts the isotropic nature of the photoelectron angular distribution which occurs due to the oversaturation of the microchannel plates of the electron detector. However, along with the oversaturated signal, the original photoelectron angular distribution is also visible (Blue arrows in image **a.**).

The raw image is loaded into MatLab as a matrix (height, width, intensity). Using the 'imtool' feature different intensity levels can be selected to extract the signal and exclude the noise.

Image **b:** shows a large intensity range.

Image **c:** noise is excluded along with some of the original signal.

Image **d:** final intensity range after extraction of the real signal from the image.

TD-DFT Results

1a) Excitation energies and oscillator strengths of ZrSi at the UB3LYP/*Single basis set* level of theory:

Excited state symmetry could not be determined.

Excited State 1: 3.064-?Sym 0.0464 eV 26720.40 nm f=0.0000 <S**2>=2.097

7A -> 11A 0.34159

8A -> 12A 0.10286

9A -> 11A -1.17209

6B -> 8B 1.16460

6B -> 13B 0.11287

7B -> 10B 0.23359

7A <- 11A 0.26992

9A <- 11A -0.96916

6B <- 8B 0.92194

7B <- 10B 0.21482

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -50.2764348937

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 4.020-?Sym 0.1183 eV 10477.94 nm f=0.0001 <S**2>=3.790

8A -> 10A 0.83110

6B -> 9B 1.03063

6B -> 11B -0.32624

7B -> 12B 0.10861

8A <- 10A 0.59341

6B <- 9B 0.67013

6B <- 11B -0.25228

7B <- 12B 0.10780

Excited state symmetry could not be determined.

Excited State 3: 3.067-?Sym 0.2138 eV 5798.03 nm f=0.0001 <S**2>=2.102

8A -> 11A -0.29904

6B -> 10B 0.10068

7B -> 8B 0.98934

8A <- 11A -0.17477

7B <- 8B 0.22117

Excited state symmetry could not be determined.

Excited State 4: 3.007-?Sym 0.4901 eV 2529.90 nm f=0.0002 <S**2>=2.010

7A -> 10A -0.39760

9A -> 10A 0.90890

Excited state symmetry could not be determined.

Excited State 5: 3.039-?Sym 0.5201 eV 2383.88 nm f=0.0000 <S**2>=2.059

7A -> 11A -0.30404

9A -> 11A 0.64290

6B -> 8B 0.70245

Excited state symmetry could not be determined.

Excited State 6: 3.947-?Sym 0.5510 eV 2250.31 nm f=0.0000 <S**2>=3.644

6A -> 10A -0.24695

8A -> 11A 0.86041

6B -> 10B -0.44186

7B -> 8B 0.24784

8A <- 11A 0.16493

6B <- 10B -0.15344

Excited state symmetry could not be determined.

Excited State 7: 3.821-?Sym 0.5623 eV 2204.95 nm f=0.0026 <S**2>=3.401

7A -> 10A 0.35264

7A -> 14A 0.10261

8A -> 13A -0.17788

9A -> 10A 0.17587

6B -> 12B 0.15116

7B -> 9B 0.89712

7B -> 11B -0.12841

7A <- 10A 0.11578

8A <- 13A -0.10645

Excited state symmetry could not be determined.

Excited State 8: 3.095-?Sym 0.6474 eV 1915.11 nm f=0.0014 <S**2>=2.144

6A -> 11A 0.18679

8A -> 10A 0.78080

6B -> 9B -0.59537

1b) Excitation energies and oscillator strengths of ZrSi at the UB3LYP/*Mixed basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 3.087-?Sym 0.0491 eV 25228.82 nm f=0.0000 <S**2>=2.132

11A -> 18A 0.10781

12A -> 16A 0.15818

13A -> 17A 0.11127

14A -> 16A 1.16726

11B -> 13B 1.17429

12B -> 15B 0.24675

11A <- 18A 0.10530

12A <- 16A 0.11564

13A <- 17A 0.10383

14A <- 16A 0.95554

11B <- 13B 0.92584

12B <- 15B 0.22667

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -335.914307416

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 4.014-?Sym 0.1917 eV 6466.69 nm f=0.0001 <S**2>=3.778

13A -> 15A 0.73742

11B -> 14B 0.88243

11B -> 16B -0.28536

13A <- 15A 0.42092

11B <- 14B 0.44396

11B <- 16B -0.19017

Excited state symmetry could not be determined.

Excited State 3: 3.164-?Sym 0.2911 eV 4258.55 nm f=0.0001 <S**2>=2.253

13A -> 16A -0.41397

11B -> 15B 0.14824

12B -> 13B 0.93918

13A <- 16A -0.19123

12B <- 13B 0.19593

Excited state symmetry could not be determined.

Excited State 4: 3.009-?Sym 0.5038 eV 2460.81 nm f=0.0002 <S**2>=2.014

12A -> 15A 0.25939

14A -> 15A 0.95722

Excited state symmetry could not be determined.

Excited State 5: 3.048-?Sym 0.5234 eV 2368.74 nm f=0.0000 <S**2>=2.072

12A -> 16A 0.21348

14A -> 16A 0.68869

11B -> 13B -0.68947

Excited state symmetry could not be determined.

Excited State 6: 3.859-?Sym 0.5612 eV 2209.33 nm f=0.0000 <S**2>=3.473

11A -> 15A -0.24319

13A -> 16A 0.82942

11B -> 15B -0.39722

12B -> 13B 0.37482

13A <- 16A 0.14028

11B <- 15B -0.13997

Excited state symmetry could not be determined.

Excited State 7: 3.093-?Sym 0.6372 eV 1945.76 nm f=0.0010 <S**2>=2.142

11A -> 16A 0.15686

13A -> 15A 0.76311

11B -> 14B -0.62379

Excited state symmetry could not be determined.

Excited State 8: 3.805-?Sym 0.6422 eV 1930.69 nm f=0.0036 <S**2>=3.370

12A -> 15A 0.39158

13A -> 18A -0.15752

14A -> 15A -0.10016

11B -> 17B 0.11606

12B -> 14B 0.89301

12B -> 16B -0.14836

12A <- 15A 0.11109

2a) Excitation energies and oscillator strengths of NbSi at the UB3LYP/ *Single basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 4.177-?Sym 0.0242 eV 51164.57 nm f=0.0000 <S**2>=4.112

6A -> 13A 0.11814

7A -> 11A 1.93470

7A -> 14A -0.11927

7A -> 22A -0.10694

8A -> 12A 0.12409

6B -> 8B 1.07662

6A <- 13A 0.11834

7A <- 11A 1.75648

7A <- 14A -0.11078

8A <- 12A 0.11729

6B <- 8B 0.90718

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -60.0156830996

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 4.171-?Sym 0.1821 eV 6810.39 nm f=0.0003 <S**2>=4.098

6A -> 11A -0.12236

10A -> 12A 0.10049

7B -> 8B 1.02624

7B <- 8B 0.26589

Excited state symmetry could not be determined.

Excited State 3: 4.069-?Sym 0.2946 eV 4209.08 nm f=0.0000 <S**2>=3.890

7A -> 11A -0.60064

6B -> 8B 0.81364

7A <- 11A -0.15690

Excited state symmetry could not be determined.

Excited State 4: 4.723-?Sym 0.4830 eV 2567.04 nm f=0.0000 <S**2>=5.327

8A -> 11A 0.95273

6B -> 9B 0.31100

6B -> 10B -0.22181

8A <- 11A 0.18732

6B <- 9B 0.12360

6B <- 10B -0.11678

Excited state symmetry could not be determined.

Excited State 5: 4.090-?Sym 0.5332 eV 2325.34 nm f=0.0002 <S**2>=3.932

9A -> 11A -0.65488

10A -> 11A 0.74974

Excited state symmetry could not be determined.

Excited State 6: 4.682-?Sym 0.8510 eV 1456.93 nm f=0.0001 <S**2>=5.230

9A -> 11A 0.73138

10A -> 11A 0.64227

7B -> 9B 0.19247

Excited state symmetry could not be determined.

Excited State 7: 4.086-?Sym 1.0480 eV 1183.05 nm f=0.0000 <S**2>=3.923

6A -> 11A 0.99000

Excited state symmetry could not be determined.

Excited State 8: 4.083-?Sym 1.1200 eV 1106.98 nm f=0.0024 <S**2>=3.917

8A -> 11A -0.31238

6B -> 9B 0.94095

2b) Excitation energies and oscillator strengths of NbSi at the UB3LYP/*Mixed basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 4.174-?Sym 0.0252 eV 49217.74 nm f=0.0000 <S**2>=4.106

11A -> 18A 0.12143

12A -> 16A 1.93858

12A -> 19A 0.13730

13A -> 17A 0.12784

12B -> 13B 1.05746

11A <- 18A 0.12144

12A <- 16A 1.75284

12A <- 19A 0.12730

13A <- 17A 0.12060

12B <- 13B 0.90102

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -345.655725087

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 4.143-?Sym 0.2589 eV 4788.14 nm f=0.0002 <S**2>=4.040

11A -> 16A -0.13766

11B -> 13B 1.01114

11B <- 13B 0.20626

Excited state symmetry could not be determined.

Excited State 3: 4.065-?Sym 0.2994 eV 4141.52 nm f=0.0000 <S**2>=3.880

12A -> 16A -0.57294

12B -> 13B 0.83096

12A <- 16A -0.14502

Excited state symmetry could not be determined.

Excited State 4: 4.719-?Sym 0.4837 eV 2563.21 nm f=0.0000 <S**2>=5.318

13A -> 16A 0.95423

12B -> 14B 0.28630

12B -> 15B -0.23861

13A <- 16A 0.18433

12B <- 14B 0.10955

12B <- 15B -0.12416

Excited state symmetry could not be determined.

Excited State 5: 4.080-?Sym 0.5646 eV 2196.06 nm f=0.0002 <S**2>=3.912

14A -> 16A -0.59103

15A -> 16A 0.80005

Excited state symmetry could not be determined.

Excited State 6: 4.720-?Sym 0.9367 eV 1323.64 nm f=0.0000 <S**2>=5.321

14A -> 16A 0.76566

15A -> 16A 0.56664

11B -> 14B 0.26316

11B -> 15B -0.12171

Excited state symmetry could not be determined.

Excited State 7: 4.075-?Sym 1.0852 eV 1142.55 nm f=0.0022 <S**2>=3.901

13A -> 16A -0.29469

12B -> 14B 0.94462

12B -> 15B -0.10408

Excited state symmetry could not be determined.

Excited State 8: 4.079-?Sym 1.0992 eV 1127.94 nm f=0.0000 <S**2>=3.910

11A -> 16A 0.98672

11B -> 13B 0.11771

3a) Excitation energies and oscillator strengths of MoSi at the UB3LYP/ *Single basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 3.420-?Sym 0.5871 eV 2111.66 nm f=0.0000 <S**2>=2.674

10A -> 11A 0.99811

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -71.2326901906

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 3.420-?Sym 0.5871 eV 2111.65 nm f=0.0000 <S**2>=2.674

9A -> 11A 0.99811

Excited state symmetry could not be determined.

Excited State 3: 3.581-?Sym 0.7479 eV 1657.74 nm f=0.0010 <S**2>=2.956

8A -> 11A 0.98913

6B -> 9B 0.11216

Excited state symmetry could not be determined.

Excited State 4: 3.858-?Sym 0.7911 eV 1567.21 nm f=0.0009 <S**2>=3.470

6A -> 11A 0.55291

7A -> 11A 0.82559

Excited state symmetry could not be determined.

Excited State 5: 3.858-?Sym 0.7911 eV 1567.21 nm f=0.0009 <S**2>=3.470

6A -> 11A 0.82559

7A -> 11A -0.55291

Excited state symmetry could not be determined.

Excited State 6: 3.768-?Sym 1.4955 eV 829.05 nm f=0.0028 <S**2>=3.300

7B -> 9B 0.86829

7B -> 14B 0.12634

8B -> 9B 0.46097

Excited state symmetry could not be determined.

Excited State 7: 3.768-?Sym 1.4955 eV 829.05 nm f=0.0028 <S**2>=3.300

7B -> 9B -0.46097

8B -> 9B 0.86829

8B -> 14B 0.12634

Excited state symmetry could not be determined.

Excited State 8: 3.751-?Sym 1.9958 eV 621.21 nm f=0.0177 <S**2>=3.268

8A -> 11A -0.12131

6B -> 9B 0.94353

6B -> 14B 0.18913

7B -> 11B 0.13323

8B -> 10B 0.13323

3b) Excitation energies and oscillator strengths of MoSi at the UB3LYP/*Mixed basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 4.083-?Sym -0.2969 eV -4176.17 nm f=-0.0000 <S**2>=3.918

12A -> 16A 0.91343

11B -> 14B -0.45736

11B <- 14B -0.21266

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -356.887387395

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 4.083-?Sym -0.2969 eV -4176.17 nm f=-0.0000 <S**2>=3.918

13A -> 16A 0.91343

12B -> 14B -0.45736

12B <- 14B -0.21266

Excited state symmetry could not be determined.

Excited State 3: 3.418-?Sym -0.2433 eV -5094.96 nm f=-0.0000 <S**2>=2.671

15A -> 16A -0.99631

Excited state symmetry could not be determined.

Excited State 4: 3.703-?Sym -0.0486 eV -25515.18 nm f=-0.0000 <S**2>=3.178

14A -> 16A 1.18191

13B -> 14B -0.54113

14A <- 16A 0.68982

13B <- 14B -0.47328

Excited state symmetry could not be determined.

Excited State 5: 3.106-?Sym -0.0070 eV -176203.45 nm f=-0.0000 <S**2>=2.161

11A -> 16A 4.23667

11A -> 30A -0.15422

11A -> 38A -0.18795

11A <- 16A 4.11730

11A <- 30A -0.15066

11A <- 38A -0.18341

Excited state symmetry could not be determined.

Excited State 6: 3.378-?Sym 0.6938 eV 1787.08 nm f=0.0000 <S**2>=2.603

14A -> 16A 0.31851

13B -> 14B 0.95959

14A <- 16A -0.18415

Excited state symmetry could not be determined.

Excited State 7: 3.153-?Sym 0.7796 eV 1590.32 nm f=0.0000 <S**2>=2.235

13A -> 16A 0.44811

11B -> 16B -0.31565

12B -> 14B 0.87018

13A <- 16A -0.22712

11B <- 16B -0.10109

Excited state symmetry could not be determined.

Excited State 8: 3.153-?Sym 0.7796 eV 1590.32 nm f=0.0000 <S**2>=2.235

12A -> 16A 0.44811

11B -> 14B 0.87018

12B -> 16B 0.31565

12A <- 16A -0.22712

12B <- 16B 0.10109

Excited state symmetry could not be determined.

Excited State 9: 3.098-?Sym 1.0965 eV 1130.72 nm f=0.0016 <S**2>=2.150

13B -> 15B 0.98471

13B -> 19B 0.12202

Excited state symmetry could not be determined.

Excited State 10: 3.091-?Sym 1.1295 eV 1097.70 nm f=0.0004 <S**2>=2.139

13A -> 16A 0.10119

15A -> 18A 0.10381

11B -> 16B 0.32345

12B -> 15B 0.92409

12B -> 19B 0.11884

13B -> 18B -0.11900

Excited state symmetry could not be determined.

Excited State 11: 3.091-?Sym 1.1295 eV 1097.70 nm f=0.0004 <S**2>=2.139

12A -> 16A -0.10119

15A -> 17A 0.10381

11B -> 15B 0.92409

11B -> 19B 0.11884

12B -> 16B 0.32345

13B -> 17B -0.11900

Excited state symmetry could not be determined.

Excited State 12: 3.106-?Sym 1.2215 eV 1015.03 nm f=0.0000 <S**2>=2.162

13B -> 16B 0.99017

4a) Excitation energies and oscillator strengths of PdSi at the UB3LYP/ *Single basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 2.987-?Sym 0.0060 eV 207031.18 nm f=0.0000 <S**2>=1.981

12A -> 13A 2.03700

12A -> 16A -0.11821

9B -> 11B 0.19905

12A <- 13A 1.77587

12A <- 16A -0.10540

9B <- 11B 0.19737

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -130.552388764

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 3.008-?Sym 0.9766 eV 1269.53 nm f=0.0013 <S**2>=2.011

11A -> 13A 0.99362

Excited state symmetry could not be determined.

Excited State 3: 3.026-?Sym 1.4853 eV 834.74 nm f=0.0000 <S**2>=2.039

9B -> 11B 0.99815

Excited state symmetry could not be determined.

Excited State 4: 3.025-?Sym 1.4869 eV 833.86 nm f=0.0000 <S**2>=2.038

10B -> 11B 0.99416

Excited state symmetry could not be determined.

Excited State 5: 3.039-?Sym 1.9753 eV 627.66 nm f=0.0026 <S**2>=2.060

12A -> 14A 0.63406

7B -> 11B 0.77015

Excited state symmetry could not be determined.

Excited State 6: 3.045-?Sym 2.1407 eV 579.18 nm f=0.0050 <S**2>=2.068

10A -> 13A 0.24652

12A -> 14A 0.74187

7B -> 11B -0.61882

Excited state symmetry could not be determined.

Excited State 7: 3.066-?Sym 2.1525 eV 576.00 nm f=0.0006 <S**2>=2.101

8A -> 13A -0.32449

11A -> 14A 0.19701

8B -> 11B 0.91667

Excited state symmetry could not be determined.

Excited State 8: 3.938-?Sym 2.1931 eV 565.34 nm f=0.0003 <S**2>=3.627

9A -> 13A 0.91842

6B -> 11B 0.15437

10B -> 12B -0.35759

4b) Excitation energies and oscillator strengths of PdSi at the UB3LYP/*Mixed basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 3.001-?Sym 0.0169 eV 73347.85 nm f=0.0000 <S**2>=2.002

17A -> 18A 1.54051

14B -> 16B -0.12538

17A <- 18A 1.17420

14B <- 16B -0.12269

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -416.196559037

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 3.013-?Sym 1.1144 eV 1112.53 nm f=0.0016 <S**2>=2.019

16A -> 18A 0.99329

Excited state symmetry could not be determined.

Excited State 3: 3.023-?Sym 1.6254 eV 762.77 nm f=0.0000 <S**2>=2.034

15B -> 16B 0.99487

Excited state symmetry could not be determined.

Excited State 4: 3.023-?Sym 1.6279 eV 761.61 nm f=0.0000 <S**2>=2.035

14B -> 16B 0.99604

Excited state symmetry could not be determined.

Excited State 5: 3.024-?Sym 1.8717 eV 662.43 nm f=0.0070 <S**2>=2.036

17A -> 19A 0.97142

12B -> 16B -0.21392

Excited state symmetry could not be determined.

Excited State 6: 3.011-?Sym 2.2965 eV 539.88 nm f=0.0012 <S**2>=2.017

17A -> 19A 0.21220

12B -> 16B 0.97325

Excited state symmetry could not be determined.

Excited State 7: 3.011-?Sym 2.3596 eV 525.44 nm f=0.0004 <S**2>=2.017

13A -> 18A 0.17226

16A -> 19A 0.28123

13B -> 16B 0.93124

Excited state symmetry could not be determined.

Excited State 8: 3.669-?Sym 2.5002 eV 495.90 nm f=0.0002 <S**2>=3.116

14A -> 18A 0.60412

11B -> 16B 0.65071

15B -> 17B -0.44150

5a) Excitation energies and oscillator strengths of WSi at the UB3LYP/ *Single basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 5.538-?Sym 0.0027 eV 455693.57 nm f=0.0000 <S**2>=7.418

6A -> 13A -0.23012

9A -> 12A -0.23464

10A -> 14A 0.11757

7B -> 8B -3.02239

7B -> 16B 0.10060

6A <- 13A -0.22974

9A <- 12A -0.23404

10A <- 14A 0.11732

7B <- 8B -2.85241

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -71.5038419833

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 5.210-?Sym 0.6572 eV 1886.49 nm f=0.0005 <S**2>=6.536

8A -> 12A 0.13531

6B -> 8B -0.99194

Excited state symmetry could not be determined.

Excited State 3: 5.049-?Sym 1.2695 eV 976.65 nm f=0.0014 <S**2>=6.122

7B -> 9B 0.99578

Excited state symmetry could not be determined.

Excited State 4: 5.099-?Sym 1.6071 eV 771.49 nm f=0.0001 <S**2>=6.249

10A -> 13A -0.17426

11A -> 12A 0.98004

Excited state symmetry could not be determined.

Excited State 5: 5.097-?Sym 1.6480 eV 752.32 nm f=0.0012 <S**2>=6.244

10A -> 12A 0.97423

11A -> 13A 0.20866

Excited state symmetry could not be determined.

Excited State 6: 5.466-?Sym 1.8787 eV 659.93 nm f=0.0000 <S**2>=7.220

9A -> 12A 0.97747

10A -> 14A -0.10720

7B -> 12B 0.15727

Excited state symmetry could not be determined.

Excited State 7: 5.422-?Sym 1.9438 eV 637.84 nm f=0.0037 <S**2>=7.099

6A -> 12A -0.14498

7A -> 14A 0.11818

8A -> 14A 0.17045

9A -> 13A -0.49624

6B -> 9B 0.67008

7B -> 10B -0.48514

7B -> 15B 0.10347

Excited state symmetry could not be determined.

Excited State 8: 5.353-?Sym 2.0328 eV 609.93 nm f=0.0065 <S**2>=6.915

8A -> 12A 0.97057

6B -> 8B 0.13172

6B -> 12B -0.12941

5b) Excitation energies and oscillator strengths of WSi at the UB3LYP/*Mixed basis set* level of theory:

Excitation energies and oscillator strengths:

Excited state symmetry could not be determined.

Excited State 1: 5.203-?Sym 0.0129 eV 96462.53 nm f=0.0000 <S**2>=6.518

11A -> 18A -0.12791

14A -> 17A -0.13056

12B -> 13B 1.75193

11A <- 18A -0.12691

14A <- 17A -0.12898

12B <- 13B 1.43928

This state for optimization and/or second-order correction.

Total Energy, E(TD-HF/TD-KS) = -357.145746122

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited state symmetry could not be determined.

Excited State 2: 5.169-?Sym 0.7394 eV 1676.82 nm f=0.0004 <S**2>=6.431

11B -> 13B 0.99343

Excited state symmetry could not be determined.

Excited State 3: 5.048-?Sym 1.1717 eV 1058.18 nm f=0.0017 <S**2>=6.120

12B -> 14B 0.99401

Excited state symmetry could not be determined.

Excited State 4: 5.086-?Sym 1.5767 eV 786.36 nm f=0.0001 <S**2>=6.216

15A -> 18A -0.18029

16A -> 17A 0.97826

Excited state symmetry could not be determined.

Excited State 5: 5.084-?Sym 1.6168 eV 766.87 nm f=0.0011 <S**2>=6.213

15A -> 17A 0.97235

16A -> 18A 0.21343

Excited state symmetry could not be determined.

Excited State 6: 5.476-?Sym 1.8649 eV 664.83 nm f=0.0000 <S**2>=7.247

14A -> 17A 0.97249

15A -> 19A 0.11741

12B -> 17B 0.17190

Excited state symmetry could not be determined.

Excited State 7: 5.377-?Sym 1.9084 eV 649.67 nm f=0.0084 <S**2>=6.979

11A -> 17A -0.11329

12A -> 19A -0.15483

14A -> 18A -0.46445

11B -> 14B 0.73442

12B -> 15B -0.44632

Excited state symmetry could not be determined.

Excited State 8: 5.386-?Sym 2.0152 eV 615.24 nm f=0.0058 <S**2>=7.001

14A -> 18A 0.53133

11B -> 14B 0.64229

11B -> 16B -0.13021

12B -> 15B 0.51438

12B -> 20B -0.10995